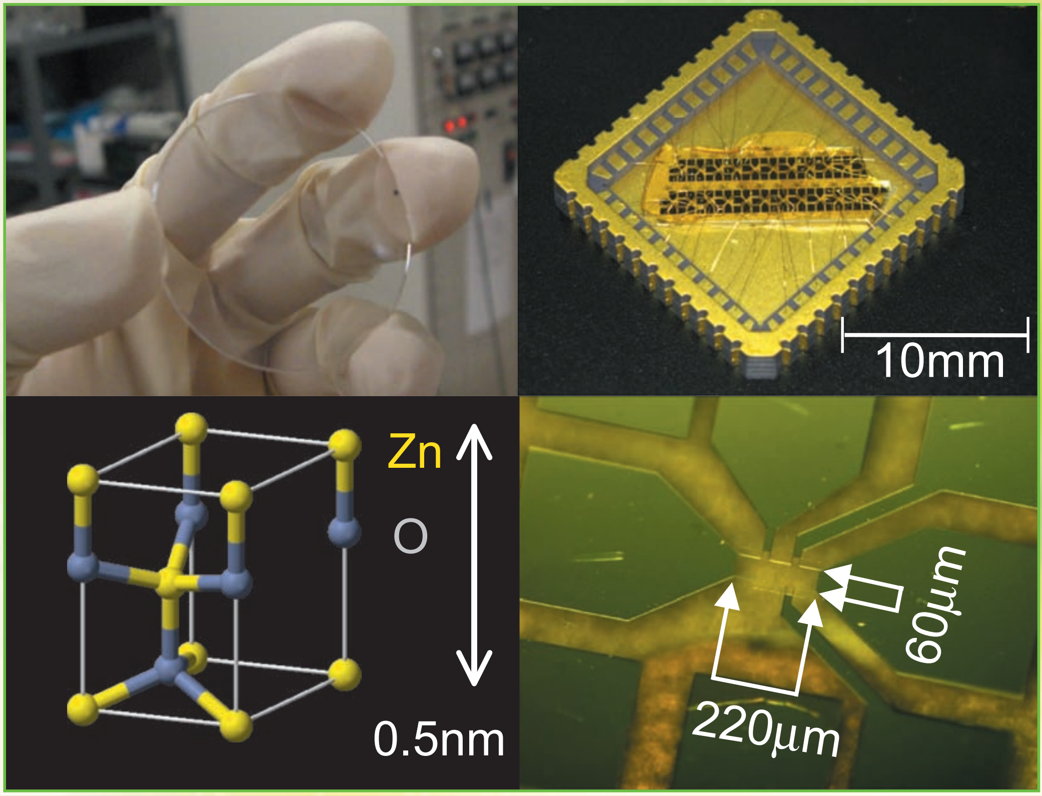
Volume 8

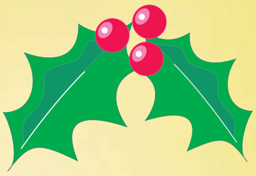
WPI-AIMR NEWS

December 24, 2009



World Premier International Research Center
Advanced Institute for Materials Research

Tohoku University



Cover: World-first quantum interference realized in an oxide device. This is called as quantum Hall effect and two Nobel prizes were given for the discoveries, in 1985 for Si and in 1998 for GaAs. Clockwise from upper left picture, 2 inches ZnO wafer, Hall effect devices mounted on a chip, a Hall effect device, and crystal structure of ZnO.

Electrons subjected to a strong magnetic field make circular orbital due to Lorenz force and interference of electron wave allows only energetically discreet states as those in hydrogen atom. In order to make it happen, the semiconductors have to be extremely clean. ZnO is a semiconductor and transparent unlike Si or GaAs. Cutting edge technology in WPI-AIMR makes ZnO ever cleanest and enables to observe quantum Hall effect. This discovery is expected to lead novel transparent electronics.

表紙：酸化物では世界で初めてとなる電子の量子干渉を観測。この現象は量子ホール効果と呼ばれ、Si での発見で 1985 年に、GaAs での発見で 1998 年にノーベル賞が授与されています。写真左上から時計回りに、ZnO の 2 インチウエハ、チップキャリアにセットされたホール効果素子、ホール効果素子の拡大図、ZnO の結晶構造。

強い磁場をかけると、電子はローレンツ力により円軌道を描き、水素原子同様電子波の干渉効果で飛び飛びのエネルギー状態を取ります。半導体でこの現象を可能にするには、極めて欠陥の少ない状態が必要でした。WPI-AIMR の最先端技術により、ZnO でも量子ホール効果の観測が可能になりました。 ZnO は、Si や GaAs とは異なり透明な半導体で、この技術により、画期的な “透明エレクトロニクス” につながると期待されます。

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Contents

Appendix

The screening process of WPI 2010 budget requests, new PIs, and others

Yoshinori Yamamoto
Institute Director

The screening process of fiscal 2010 budget took place in November in Tokyo. The task force for the "Government Revitalization Unit" recommended a significant reduction in the budget requests. A 30 %, 50%, or even 100 % reduction was recommended for some of the projects. The WPI project was not an exception, and the conclusion of the team was that "the budget requests for WPI program should be reduced." However, the team did not specify concretely how much the budget should be reduced.

The final decision by the Hatoyama Administration will be made before the end of the year. Accordingly, by the time you receive this WPI-NEWS, we may have the final judgments.

I would, nevertheless, appreciate any efforts to submit your written opinions/comments on the screening process to MEXT (Department of Education). I do hope that such comments would exert a strong influence on the decision of the Cabinet and MEXT.

I am happy to report that three new PIs have joined us by November 1 this year; Professor Winfried Teizer from Texas A & M University, Professor Ali Khademhosseini from Harvard University Medical School, and Professor Hongkai Wu from the Hong Kong University of Science & Technology. They set up research laboratories here at WPI-AIMR and pursue research with newly-hired APs, PDs, and/or students. The major research area of WT is PhysBio, that of AK is BioMEMS, and that of HW is ChemBio, so I hope that we will be able to strengthen our research regarding Bio-materials.

The present status of WPI-AIMR on the number of researchers and administrative staff is shown below. We are approaching the final goal, which was set at the time of inauguration. The ratio of foreign to Japanese researchers is 58% and this is far beyond the percentage (30%) requested by MEXT. The structure of our organization is now in good shape, but much more important are our accomplishment in research and how those accomplishments are innovative and influential to the scientific community and to mankind. I believe that this primary mission for us is proceeding well.

	Planned Final goal	2007	2008	2009 As of December
Principal Investigators	30	30 (12)	29 (11)	32 (15)
From **Tohoku Univ.**	15	15	15	15
From **abroad**	11	11	10	13
From **domestic**	4	4	4	4
Other Researchers (Associate-Prof, Assistant-Prof, PD)	90	12 (4)	54 (22)	83 (52)
Research Support Staff	53	1	13	41
Administrative Staff	40	16	26	29
Total	213	59	122	183

( ) --- foreign researchers

Interviews

Interview of Professor Herbert Gleiter, Institut of Nanotechnologie, Forschungszentrum Karlsruhe & International Advisory Board, WPI-AIMR

"Enjoy free discussion with imagination"

---Curiosity is the root of science---

Prof. Komatsu (K): Please start with what sort of family or where you were born and your childhood.

Prof. Herbert Gleiter (G): Well, I grew up in Stuttgart which is located in the southern part of Germany.

K: Stuttgart? A very big city.

G: Well, not on a Japanese scale. About half a million or three-quarters of a million citizens ie. smaller than Sendai.

Concerning my background, one can find two groups of people in my family. One was a management-type background. For example, my father was a manager of a bank. This is the one side. And then some of my relatives had a science or an engineering background. In fact, a unit is named by one of my forefathers. As you probably know, if one produce wine, one starts with the sweet juice from grapes. He noticed that by measuring the sugar content of the juice of the grapes, one can predict the alcohol content of the wine. His name was Oechsle. Today, the sugar content of the grape juice is measured in degrees Oechsle. He was my grand-grandfather.

If one goes through the generations, one can find people doing more business-type things and then others involved in science. In fact, my brother for example is a professor at the University of Heidelberg. He is in chemistry. Not far away from what I am doing. My son is not in science.

K: That's interesting.

G: Yes. In my case I can say that I was strongly coined by the people I met as a student. I studied at the University of Stuttgart and received my Diploma Thesis as well as my Ph.D. Thesis at the Max Planck Institute for Metals Research at Stuttgart. There I worked with Professors Koester, Seeger, Dehlinger and Hornbogen. These colleagues had certainly a strong influence on my education.

K: Very famous colleagues.

G: Yes. If you look at my CV, you will notice that I studied first mechanical engineering, and I finished mechanical engineering with the Diploma degree. During my studies as a mechanical engineer, I discovered that this field covers my interests only partially. I was more interested in questions closely related to physics. This was the motivation for me study subsequently physics. I obtained my Ph.D. in physics.

First I thought studying two fields was a loss of time. However, later in my life, when I became one of the presidents of the Research Center at Karlsruhe – one of the two largest National Laboratories of Germany - I discovered that my two backgrounds in mechanical engineering as well as in physics were most useful. As a president of a research center with a size of several thousand people, one is faced not only with questions related to science but also with management or economic aspects. These aspects are better covered by an engineering education than by an education in physics.

K: But before you focused on your target of study, how did you get your interest in engineering or science when you were a boy?

G: Essentially it was the people I met when I was a student. I met several people who impressed me, for example, Professor Dehlinger was one of them, or Professor Hornbogen or Seeger or Koester. Professor Koester was the director of the Max Planck Institute of Metal Research at Stuttgart at that time. And it was by this background, this personal contact, that got me interested in the field of materials science and solid state physics.

K: Why did you choose physics or science instead of literature?

G: It was the way of thinking in physics. Actually, I noticed this preference already when I was in school.

K: Even in childhood?

G: Even in childhood. In fact, together with my brother we performed experiments in physics and chemistry.

K: You were influenced by your brother?

G: We both did these experiments together. We had to buy chemicals, instruments, equipment etc. and then tried to perform the planned experiments together. And I still can remember when we did one of these experiments. My father and my mother had to be off at a business meeting of my father. We used that opportunity for some experiments. Something went wrong and we started a fire. After a short while one of the curtains started to burn. At that moment my parents returned. You can imagine their reaction. They stopped us for a while with our experiments.

K: We are interested in such things.

G: It was this experience to see something to happen and being able to understand it. For example, if there is a chemical reaction, to understand why it exists.

K: It’s very funny. That famous Richard Feynman also had the same experience.

G: It’s a strange thing, indeed. It’s irrational but it seems to be part of our personality and it was this experience that triggered my interest in the field. Sometimes in school, I had some problems with this facet of my personality. I openly said, in which fields I was most interested in and also made it clear what areas were of minor interest to me. Unfortunately, some of my teachers, in humanities, for example, were very influential, and they didn't like this kind of attitude. However, finally I got my "abitur" degree that allowed me to enter university.

Clearly, for me the driving force to work was primarily curiosity and interest. The same applied to my activities during my university education. I was interested in a subject or I was excited by people who represented a field. I had the same experience later when I was a post-doctoral fellow at Harvard and at MIT. There were people like Bloembergen, Cahn, Orowan, Argon, Turnbull or Chalmers.

K: You've been to Harvard after graduation?

G: I've been at Harvard, first for three years and then one year at MIT.

K: Orowan and Turnbull were there?

G: Yes, they were there. Turnbull's office was very close to mine.

So I knew all of them. Chalmers was there as well. It was important for me to talk to these people and discuss with them what I was doing. Also to see what they are interested in. Every day after lunch we had a coffee break. Most of the members of the faculty attended. And then one could talk about what one was interested in. And they told us what they were doing or planning.

K: Every day?

G: Every day.

K: After lunch together? That was very nice.

G: I think that was the most important time of the day, at least for me. You can go to lectures everywhere. However, talking personally to people and also getting their response when you have an idea, this is what you cannot get at a conference.

K: A very informal way?

G: Yes, very informal.

K: Anything you could ask and discuss.

G: Yes, anything. Many years later, when I became a professor at a university, I used to have the same tea break after lunch. When I left university and went to Karlsruhe, as a president of the Karlsruhe Research Center, I asked about 20 of my former students (who had become professors when I asked them) what they would consider as the most important factor in their education. They all told me that it was the tea break after lunch. We sat together and we talked about the things we were doing or planning.

K: That is the same idea I have. In England I learned how important tea time is.

G: It’s a very important portion of education. One is relaxed and one can talk openly. And also, I noticed that some students did not speak up. This is frequently a sign that something goes wrong. Some are shy if they have problems and hence they would not speak to you. However, by watching them one can find out if something may be wrong. If a student doesn’t participate in the conversation then that may be a signal that you better talk to him or her. On the other hand, at an official presentation e.g. at a conference, he or she would sit quietly and one would never notice that they may have a problem.

Another aspect is that the relationships that originate from that time last over many decades. Even today, when I need some information or some help, I can just call former students in the States or anywhere else and they tell me honestly what they know. So this human aspect is very important in science as well.

K: Yes, it is.

G: I think it was Heisenberg who said we should always keep in mind that science is done by people. Science is not independent of people.

K: It’s very deeply rooted.

G: Yes. Science and scientists are intimately related.

K: Yes, yes, indeed.

G: I think this is what is often overlooked by people in politics.

K: That’s right. They don’t know.

G: I mean, research plans and programs are all meaningless, unless you have the right people.

K: Politicians often know only the final result.

G: That is true. And that was also my view, when I started the new institute called “Institute of New Materials” at Saarbrucken and later the “Institute of Nanotechnology” at the Research Center Karlsruhe. I always tried to build the institutes around the people. At Karlsruhe, initially we had eight people. They knew each other already before the institute was founded. The idea of that institute was to form a research institute bringing together scientists who have a background in physics or chemistry or engineering either in theory or in experiment. All of them had already an institute at a university. What I did was nothing else but bringing them together and providing them with additional money, additional space, and additional positions. In other words, we provided them with the means to pick up new ideas or to form new co-operations.

K: Different specialties.

G: Yes.

K: Interdisciplinary discussion and co-operations among colleagues.

G: Yes, this is what it was.

K: This is very productive.

G: And they had plenty of opportunities to talk to each other and to the students. We were very fortunate that we found for the Institute of Nanotechnology a Nobel Prize-winner and four Leibniz Prize-winners. Having outstanding scientists in such an institute is important in several respects. First of all for the reputation of the institute. However, also for the students. They can see that famous people also are not protected from making mistakes. This is very important. If a student makes a mistake, he should not think that he is stupid and the professor is wise.

K: Yes, human beings.

G: We are all human beings and everybody is allowed to make mistakes.

K: Yes, so they can discuss openly.

G: Yes, yes. And ask good questions.

K: Yes, that's right.

G: I think this is important. Because when one is a student, in the beginning one only reads textbooks and everything is clear. Then one starts doing research and soon one discovers that one keeps making mistakes. As a result, one has the feeling - at least I had the feeling – that I am stupid and everybody else never makes mistakes. Naturally, later on one discovers all the other people make mistakes as well. It's only that some people occasionally are very successful, and this is what counts.

K: Yes, yes.

G: History of science teaches us that the mistakes a scientist made are forgotten. He will be remembered for the important contributions he made. This seems to be an important observation we should teach to the student. In fact, mistakes are sometimes necessary to open the way to progress. And that's why - when I had to teach at the universities - I copied papers from famous people where famous people said something that turned out to be wrong, and also how they found out later that it was wrong. I

handed out those publications to the students. A famous person can also make mistakes, but that's not important because later on he/she did something which was important and for that publication we know him/her. So don't be afraid of making mistakes. Do not hesitate to try something risky. If you fail it doesn't matter. It's far better than not trying.

K: That's right. It just also happened to Prof. Yukawa who won the Nobel Prize for the first time in Japan. After he won the Nobel Prize he became a director at a theoretical institute. He had a lot of serious, silly questions and the students were surprised that such a Nobel Prize man is asking such very silly questions.

G: Asking silly questions is okay.

K: We don't mind.

G: Yes, exactly. That's the way you get going. I mean, if you look at many discoveries, they started with silly questions.

K: Yes. And imagination is also very important.

G: Yes. And I remember when I started to pioneer nanocrystalline materials, this work started by asking the following straightforward question. Conventional polycrystalline materials consist of crystals with a diameter of e.g. a micron up to many millimeters. These crystals are connected by interfaces with a thickness of a nanometer or so. In other words, the volume fraction of the interfaces is negligible in comparison to the volume fraction of the crystals. My work leading to nanocrystalline materials started when, I turned the situation upside down and asked the question: What kind of material do we get if we create a solid with comparable volume fractions of interfaces and crystals? In order to get this kind of structure, we had to reduce the size of the crystals to a few nanometers i.e. a few interatomic spacings. We tried it in various ways and after a short time it worked all right. When we had this new class of materials, we started to study them. After we had our first results, I gave a talk about them. I think it was at a special event of the German Metal Society. In this first talk, I explained the basic idea and what we knew already about this new class of materials. After I finished my presentation, the president of the German Metal Society got up and said very loud: he is all crazy, such things do not exist. All I could do was to remind him that we have such materials already and that they are fairly stable.

But even if the speculation about the structure and the properties of these new materials would have been wrong, at least it would have been worth to try to generate them. And that was something that I have learned from Dave Turnbull. If one had an idea and explained it to Dave Turnbull, Turnbull thought about it, then he came back the next day or so and said, this portion of your idea, I think, is correct and this portion seem wrong - why don't you think again about this kind of thing? He never said, don't do it.

K: A very good man.

G: Yes I admired Turnbull.

K: There are so many eminent scientists under his guidance.

G: Often it is worth to try something. And one discovers that things work out in strange ways.

I think for a student it's important to be encouraged. He should realize that he is younger but he should never have the feeling that he is inferior. Quite often people believe that a famous man only poses very good questions or is very wise. This is all nonsense. He also makes mistakes.

And I think it is often the media which generate the impression e.g. if somebody is a Nobel Prize-winner, all of a sudden he makes no more mistakes.

K: That is not possible.

K: Your work as a student was on nanocrystalline materials?

G: No. When I studied physics at Stuttgart at the Max Planck Institute I performed some theoretical work during my Ph.D., and some studies by electron microscopy to check if the theory was correct.

K: You did both theoretical and experimental work.

G: Experiments during my Diploma Thesis. The Diploma Thesis was experimental and the Ph.D. was mostly theoretical work on dislocation theory and the interaction of dislocations with precipitates. This work brought me to the States, because I did this work at a time when dislocation theory became available and people knew empirically about what is called today superalloys. These nickel-based materials were used frequently at that time e.g for turbine blades of jet engines. However, it was not fully understood why these materials have high strength at high temperatures. By applying electron microscopy we could see the dislocations and we could see the precipitates as well. This opened the way to study the interaction between the dislocations and the precipitates, and that knowledge allowed us to understand and even predict the properties of these alloys and optimizing their properties. And that's the way I got to know other people like Bernie Kear. He was at that time a director at the research laboratory of Pratt-Whitney. Pratt-Whitney was a company that was building jet engines. He became interested in my work on precipitate hardened alloys and invited me to the States.

K: That was in nineteen sixty-something?

G: That was in '67.

K: When I went to Bristol in 1965 there was Dr. Thompson who is known for example by the "Thompson tetrahedron."

G: Yes, of course.

K: The good old days.

G: So you must have also met Frank, Charles Frank.

K: Of course. Every day I met him at tea time.

G: Yes.

K: Frank was quite a character and he was fond of looking at photographs taken by phase contrast microscopy to observe the very small steps of the surface.

G: That was at the time when Frank was interested in diamond?

K: Yes. And he often looked at a picture for one hour or so, just saying nothing. Quite a remarkable man.

G: I had a similar experience with Dave Turnbull. I can remember there was once somebody who gave a talk at Harvard. In this talk he criticized Turnbull very badly, and Turnbull was sitting there and he said nothing. Later I asked him, Dave, why didn't you say anything? He said, well, if he is correct, there is no point in saying something, and if he's not correct, it will turn out anyway. I learned a lot from Turnbull.

K: Very interesting.

G: Yes. Chalmers was totally different. He was more outspoken. If he didn't like something, he expressed it very frankly. He had no problem in saying openly: what one just explained does not seem to him to be correct, and he then walked away. In fact, I can remember one such case. We had a visitor. He came—I think from Russia—and Bruce Chalmers was standing together with him and me. The visitor told us what he did, and then we talked about it again and he apparently had told us things twice. All of a sudden Chalmers walked away without saying anything. Later I asked him, "Bruce, why did you walk away? That wasn't too polite." He said, "Well, if he tells me things twice, he must think that I am stupid."

K: I see. So two famous professors, Chalmers and Turnbull. In the same department?

G: They were in the same department, right next to each other. And at MIT it was Orowan. You probably know him because he was one of the scientists who discovered the dislocation.

K: Orowan, yes. He proposed the edge dislocation.

G: Yes. What was his background?

K: He had a technically oriented background; different from physics.

G: Yes, that's right. He was an engineer and he worked at Berlin. He told me how he came from Hungary to Germany.

K: Oh, yes.

G: And he worked at the Kaiser Wilhelm Institute at Berlin, and that's where he performed studies on plastic deformation. In one of our many meetings after lunch or dinner, he told me how he discovered the dislocation. He dropped a crystal and he noticed the slip lines and found out that these lines represented step at the surface. This observation made him think how that could happen. He then tried what happens if one shears a regular arrangement of elastically deformable spheres. In fact, he noticed that layers of these spheres do not ride simultaneously above one another. They shift by moving one row of spheres at a time. These observations were essential for him to propose the idea of a dislocation.

K: He's in a way a self-made person, learning by himself a lot.

G: Yes. That's right. He was one of the most brilliant and broadminded people I have met. At the same time he was very outspoken. He either liked a person or he didn't like him. If he didn't like a person, he didn't talk to him. It was a strange thing. But he was a very special person in the sense that he had a broad background. Of course, he knew that I came from Germany. We had plenty of time to sit together. He told me about his experience in Germany and in England. He also explained why he left England again and went to MIT. At the time when I met him, he was interested in economy.

K: Oh really?

G: Yes. When I told him what I was doing, he listened to it, but his main interest was economy at that time. He thought that it would be possible for him to contribute something of basic importance to economy. He thought that in physics many problems were already solved, and so he preferred to go into economy. Some of his colleagues had either a very positive opinion about him or a negative one. The way he approached people was different from the conventional way. In addition to Prof. Orowan, there was another impressive scientist at MIT. You might know him. It was John Cahn.

K: I met him. He visited Tohoku University.

G: I see.

K: In which department was he?

G: He was in the Materials Science Department.

G: He was for many years at MIT. And then he went on to NIST, National Institute of Standards at Washington. He's now retired and lives in the State of Washington.

K: Is he still alive?

G: Yes, he still is alive. A very active person. I met him recently at a conference organized by the National Academy of Engineering.

K: And he put forward a theory about crystal growth from the melt.

G: Yes, that's one of the contributions he made. Of course everybody knows his important contributions to our understanding of spinodal decomposition, to the understanding of surface tension and to the stability of interfaces.

K: Yes, that's right. We tried to prove his theory by our experiments.

G: Yes. He was an exciting man to talk to. He had a very broad background. He was also born in German and his family had to leave Germany. Sometimes people confuse him with Robert Cahn in England.

K: He lived in Sussex.

G: Yes, he lived for many years in Sussex. He visited in the 80's and 90's quite often my institutes at Saarbruecken and at Karlsruhe respectively. We had many common interests and hence we developed a close relationship.

K: I see. He also visited the INM (Institute of New Materials)?

G: Right.

K: And we had a close relationship with him.

G: Robert Cahn made important contributions to the understanding of recovery and recrystallization. Moreover, he is one of the editors of the famous textbook on physical metallurgy

K: Oh yes.

G: Three volumes.

K: Physical metallurgy?

G: Right. That was Robert Cahn. He knew a lot of literature. Often, when I had a new idea, I sent it to Robert and got his comments. I had a similar experience with Orowan. When I told Orowan about a new idea, he sometimes quoted people from the 18th century. You know, he knew old portions of the literature, I was not aware of.

K: He knew historical things.

G: Yes.

K: Arts as well. He was a very broad person.

G: Very broad, yes, very impressive. And he had often a very special view and opinion. He had his own way of thinking and of looking at things, and I learned a lot from him.

K: He wrote his autobiography and it was translated by a friend of mine into Japanese.

G: Ah, that reflects him.

K: Very interesting.

G: Oh, I gained a lot from all of these people.

K: So the people you are talking about are quite familiar for me, from 30 or 40 years ago.

G: Yes, now I'm getting older.

K: We are all getting older.

G: Yes. But there is one thing I learned from this experience: science is not decoupled from people. It depends very strongly on to whom you talk. In a way, it's like a resonance effect. You have to talk to the right person at the right time in order to get the information or the stimulation you need to develop a new idea.

K: Actually, one of the purposes of this interview is to show that a scientist is not a unique person. A scientist is a very human being.

G: Yes. Heisenberg emphasized that science is done by people; never forget that.

K: Really? He said so?

G: Yes, Heisenberg, many times emphasized that. Science couples to people and is coined by people. This insight also comes up in the so called Harnack principle of the Max Planck Society. The Max Planck Society tries to build an institute around the person and never have a structure and try to find a person that fits into in the structure. And I think that was very successful.

K: I see.

G: Unless you have such a person that coins a field it is hard to create a world class institute.

K: The building itself is only the house to provide the research conditions an outstanding scientist needs.

G: Yes. They try to get excellent people. Often, they close an institute once the person dies or retires.

K: They keep their things.

G: This is what many politicians cannot understand. It's not the structure, it is the person that is most important. The structure is necessary but not sufficient. You need a special person.

K: They cannot see. The action of scientists cannot be seen from outside, so politicians don't know what scientists are thinking and doing.

G: Yes. In fact it is the same thing I noticed, at the time, when I was at Harvard. At that time X-ray studies on the structure of DNA were performed. Collaborators of Watson and Crick used our x-ray facilities, and again, it was the people who were most important. It was not the X-ray instrument. Naturally, concerning the equipment, the experiments could have been carried out somewhere else. It was this group of people that did the work.

K: Very interesting.

G: This is what I think young people should keep in mind.

K: Yes, indeed. So perhaps next, let’s go to the exciting findings.

G: Yes, this was the nanocrystalline material. I think we have nowadays several thousand publications a year on these materials. I’m often asked, why did you do this? And people always imply—or at least, people who are more outside of science—that it was the idea to make something useful. This is not true. It was just curiosity.

K: Curiosity. That’s very important.

G: Yes. I was working on interfaces. We studied them by taking two big crystals and had one interface between them. This work was partially performed during my time at Harvard. When I went back to Germany, I thought about the question: what would happen if we introduce more and more interfaces into a crystals?

K: So, this was purely out of curiosity.

G: Pure curiosity. Yes. In order to get more and more interfaces into crystals, we made the crystals smaller and smaller. Finally we arrived at a size of the crystals of a few nanometers. In other words, our crystals consisted of relatively few atoms only.

K: And how could you make it so small?

G: Well, we made it by a technique which I learned in Greenland. When I was a student I went to Greenland, on the inland ice cap. And when one looks at a thin slice of this ice in the light microscope, one can see that inside of the ice there are numerous very tiny dust crystals which came down from the atmosphere together with the snow that formed the ice. These tiny crystals are embedded in the ice. Of cause, these crystals cannot grow because they are surrounded by the ice.

So, we utilized the same structure, I have seen in Greenland to produce the nanometer-sized crystals which we needed to get the large volume fraction of interfaces in our material. Our equipment consisted of a bell jar with a cold metallic plate inside of the jar. Water vapor was leaked into the jar. This water vapor formed a thin layer of ice on the cold plate. Then we started to evaporate gold inside of the jar, the gold condensed in the form of nanometer-sized crystals on the ice. These tiny gold crystals got frozen into the ice. So in the end, we had ice which was black. It was black because it contained many tiny gold crystals. Finally, we sublimated the ice, collected the gold crystals, and consolidated them at pressures of several Gigapascals. This was the way how we got the first nanocrystalline materials.

K: Very interesting.

G: But the idea how to produce them was from Greenland.

K: I see. Have you ever published this?

G: Yes, that was published.

K: How about your idea initiated by your time at Greenland?

G: No, I never mentioned it in a publication.

K: It often happens. For instance, Prof. Nakaya, who grew artificial snow crystals for the first time in the world, he studied the shape of snow crystals and took many beautiful pictures under the microscope, but nobody knows how he could manage to set the snow crystals under the microscope. It was very simple. He put saliva on the tip of a matchstick and fixed a snow crystal.

G: And you just take them off.

K: And he didn't write it, so a lot of people asked, "How can you catch and set snow crystals?" Nobody knows the secret.

G: From the outside it looks magic. Infact, it is not. However, this is how things often work. Once we had this knowledge, it was easy to get these tiny crystals. Normally if one produces crystals, they keep growing all the time. The same happened in our experiments in the beginning. And then I recalled the tiny dust crystals in the ice of Greenland. This opened the way to the nanocrystalline materials.

Very soon, some of our early equipment will be exhibited in the German Museum of Technology at Munich. This museum tries to collect and exhibit equipment that was used in the past by people who are known today for their contributions to science and/or technology such as, for example, the first gasoline car by Benz or Roentgen's X-ray equipment etc. The museum collects all these historic pieces of equipment, so that people can see how discoveries are made. I think it is important that people see how new ideas develop. Very often the picture of discoveries conveyed by the media to the public deviates considerably from reality.

K: That museum must be very famous for science and technology.

G: It's like the Science Museum at Chicago. However, it is probably larger in size and certainly older. Hence, they had the opportunity to get the first light microscope, the first electron microscope from Ruska, or Lilienthal's air glider etc.

K: Kept in that museum?

G: They keep it in the museum and they show it to people.

K: Oh, very interesting.

G: And they also have our first piece of equipment that was used by us to produce the first nanometer-sized gold crystals following the method I learned from the ice in Greenland. They are preparing at the moment an exhibition on Nanoscience and Nanotechnology. This exhibition will open in November 2009. One section of this exhibition will be on nanomaterials. In this section it will be explained that the driving force for this development was curiosity. In this exhibition they will also show this

funny looking piece of equipment, we had used in the beginning to produce tiny gold crystal embedded in ice. This piece of equipment looks a bit like a Christmas tree.
As I explained already: what we used was an evacuated bell jar and a cold plate that was kept at liquid nitrogen temperature inside of the jar. Into this bell jar we leaked water vapor. The water vapor kept freezing onto the cold plate so that it turned white. Above the cold plate we had a vertical rotating stick with horizontal arms. From the ends of these arms we evaporated the gold from small tungsten boats. During the evaporation process the stick with its arms kept rotating so that it looked somewhat like a rotating Christmas tree

K: You made it.

G: We still have it and that will be shown there.

K: But a long time ago.

G: That was in 1975 or so.

K: I see.

G: Yes, that was the first approach to produce these nanocrystalline materials. And some people came and saw it and they frequently asked us: what are you doing here?

I remember on of these visits when I was at the University of Saarbrucken. At that time I was awarded the Leibniz Prize. The Leibniz Prize goes along with 5 million euros of research funds. One of the attractive features of this prize is that you can use these funds in whatever way you like without writing first proposals etc. After I was awarded this prize, the minister of research visited our laboratory. When he saw this rotating “Christmas tree”, he had a problem understanding that this could result in the award of such a prize with such a high reputation.

K: Yes, that is very good for the younger generation to see.

G: Yes.

K: The initiation of new inventions.

G: And how things develop. Yes.

K: Yes, I how things are developed, yes.

G: They don’t develop like in the textbook.

K: No, not at all. The textbook is too purified and simplified.

G: I can remember, when I was one of the presidents of the Karlsruhe Research Center, I had to talk often to the Federal Minister of Research and Development. This minister was a lady. She kept emphasizing that for good research you need first of all a network, and secondly, you need a research plan, and finally you have to define your research goals before you start.

I kept telling her, when Columbus took off for his first famous voyage, he had no network, he had no research plan, and he did not have the goal to sail to America. But he brought something back.

K: Yes, he did.

G: That's the difference.

K: Very good.

G: Yes, development is different from research. One can develop something, like improving a car or designing some kind of equipment if one knows the underlying physical principles. In order to do it, one can make a plan and one will be successful in many cases. However, development a totally different thing from research. In research one may discover something or one may fail. And apparently people who have more of an administrative background, they don't like this kind of uncertainty.

K: But uncertainty is the source of science.

G: That's the only way we can do it. Yes.

K: There is no need for any kind of study if we understand things already.

G: This view is also supported by the results of the Leibniz Prize. The Leibniz Prize exists now 25 years. Every year 10 scientists are selected from all fields of science to receive the prize. When this prize existed 20 years, a study was made on the achievements of all the people who received the prize within these 20 years. The achievements were evaluated by using generally accepted criteria of scientific quality such as other prizes and awards received by the Leibniz Prize winners in the years after they were awarded the prize, offers of directorships etc. at other institutes, the same criteria as are used by the citation index, and five other criteria, such as the number of Nobel Prizes awarded in the subsequent years to the Leibniz Prize winners etc. These criteria were normalized that per unit of money spent on research by the Leibniz Prize winners in comparison to the research funds spent by individual proposals approved by the German National Science Foundation (DFG) and also with group proposals approved by the same institution.

This evaluation revealed that the Leibniz Prize (which requires no proposals, no research plan, and no network) resulted in about 20 times more results per unit of money (measured in the above criteria) than by group proposals and about 10 times more than by individual proposals. This result tells us something about funding methods in science. It suggests, if we give a good scientist time and money, he/she will try to be successful. Moreover, not a single one of the Leibniz Prize winners misused the money. Not a single case! This teaches us that all this controlling by the administrations may not be very useful in the sense that we get as much as possible for the research funds we have spent. I am afraid the administration required to prevent the very few cases of misuse is far more expensive than the money it saves. We should accept that good scientists are interested in what they are doing and they are not interested in misusing funds, at least in science and in engineering.

But this is something I think which is not so easy to understand for other people in the administration, it seems.

K: Particularly politicians don't understand it at all.

G: Scientists are a bit like monks. Aren't they? They are interested in what they are doing and not all in the public attention. It is unfortunate, that many people cannot understand it.

K: It's very interesting.

G: That's why I always try to advocate this attitude in my function as one of the vice-presidents of the National Academy of Sciences of Germany. Give good people freedom, don't constrain them by administrative measures and you will get the maximum output for your research funds.

K: That's right.

G: We will get the more success the more freedom we give them. Unfortunately, politicians hear the words but they cannot believe the message or they do not understand it. This view is supported by many of the big discoveries. They were not planned. Consider as an example the discovery of the X-rays or of general relativity or of quantum mechanics. In fact, I got recently interested in quantum mechanics. For that reason, I read Planck's original publication again. In doing so, I noticed that he mentioned that the concept he proposed in his original publication is a model for calculating the observed emission spectra. However, the underlying physics may be quite different. We still have to try to understand the physics behind Planck's idea, as was emphasized by Feynman.

K: One arrives at the same conclusion if one looks at the discovery/development of our understanding of electricity or ferromagnetism. It was always curiosity.

G: It's curiosity.

K: When Faraday published his results on electromagnetic induction, people asked, "What is the use of it?" And Faraday said, "Can you say to young people or a newly-born baby, what he will be, what is his talent? Can you say that about this baby?"

G: Yes. You never know. However, one knows, that in the long run, without science we will have no progress. And the funds we spent on science and technology correlate with our standard of living. A high standard of living correlate with large amounts of money spent on developing science and technology. That's all we can predict. But we cannot say, I do this and that and tomorrow you will have a patent. This is nonsense.

K: Nonsense.

G: Yes. Moreover, life would be boring if it were so. As you know, it is curiosity what makes life interesting. In that sense, we are a very special class of people, I think.

K: A very, very good story. So the principle features in research have almost all been said.

G: Yes, I think so. In a way I was very fortunate because all my life I could do those things I was most interested in. It's of course a huge privilege. The salary was a kind of side product, if you wish. If I would have wanted a higher salary, I could have stayed in engineering. As an engineer I could have joint a big company, and tried to become a manager or a president of a company. In that position I would have probably received a higher salary than the one I was paid as a professor.

K: But you were interested in science itself.

G: Yes, for me the highest priority was my interest in science.

K: And doing science for your happiness.

G: Yes. And quite often, if one thinks about it, one doesn't feel that doing science is work in the sense as it is defined by most people. As you know, we are mostly "time-controlled." It's the time that limits what we can do. Even if we would have more money, we could not do more things, because we would not have more time. Isn't that true?

K: Yes, time is a limiting factor.

G: We only need so much money that the money does not constrain what we do. However, this limit is mostly fulfilled if we earn say 100,000 € or so per year. Ten million or a hundreds million euros would be meaningless in that sense; one can't use it. I never understood why people wanted to get a salary as high as that. These huge amounts of money may even yield negative effects. They take our time away because managing such amounts of money is a full time job.

K: That's right.

G: Actually, it creates a lot of work, to manage a million or even a billion, doesn't it? So it's a negative effect rather than a positive one, if one applies the above criteria.

K: I think it would be.

G: I think it's true. All the countries with high standards of living spend considerable funds on research. But the public is told by the media that we do research because we want to earn high salaries. It's a strange thing; in a way it couples into the structure and the system of values of the society. In fact, the opposite seems to apply as well: countries that do not spend much on research and education, do not get out of poverty. This is what you can see for example in Africa. As you probably know, Africa is a rich country if you consider their resources in raw materials and in people. They have land, they have people, nevertheless the country remained poor so far. They spent little money on education and research. Japan I think is an example for the opposite development. After the Second World War, Japan developed at a remarkable pace. They spent large amounts of money on research. And the Chinese people are now doing the same thing.

However, if we point that out, it is always a bit provocative for the politicians. They tell us: do you want to teach us how we should run a country? I keep saying it occasionally in small committees. However it makes a difference if you say it under six eyes or say it under 600 eyes. We have the responsibility for the institutions we represent.

K: But science, a lot of science is very deep and needs a long history. For instance, the development of Japan—modern Japan—started more than 130 years ago when the Edo era changed. They spent a lot of money just for education, reading books and counting simple things. So the number of illiterate people in Japan became almost zero in the 20th century. That was the background to develop modern science. So it took many years and huge manpower to level up the education.

G: Yes. Today, the situation is, of course, different because the turnover time became much shorter than it was say100 years ago. Nevertheless, the basic arguments and the background are still the same. For example, consider China. As you know, in ancient China high education had always a high value. And it still does. When you go to the United States, the Chinese succeed very well. One reason seems to be that the families offer their children a good education. Whereas, many of the people that live in slums, do not realize or want to realize that one way out of the slum is education. Of course, education goes along with hard work. I was reminded of this correlation when I was in Singapore recently. The Government of Singapore published a paper discussing what distinguishes people in the United States who are successful from the people who are not successful. What they found out is the following. If in a family education has a low value, then their children have less success. The opposite applies as well. It's not only the background in knowledge. It is also the general attitude. And I think this is one o f the reasons why Singapore does so well economically. Here education has a very high priority.

K: And before the war in Japan, scientists or teachers were very much respected and people looked down on money.

G: Not anymore? Now their standing is changing? But still they have high respect, don't they?

K: Moderate respect to Science in modern Japan.

G: Yes. I think this is important, because it attracts young people to these fields. Moreover, it helps to decouple interest from income. Income is one thing and interest is another thing. And this respect is something which excites young people to do something. It's not the money so much. There is a different attitude. Otherwise, you end up with a country full of managers but there is little left to manage.

K: The time is almost up. So your message to the younger generation please.

G: The same as I said already: Do what you are most interested in and you will do it best.

K: Yes. That's what you've said, yes. Okay, almost finished. What sort of hobby do you have?

G: Oh, that depends on my spare time. In recent years it's sailing on the ocean.

K: Oh really. When did you start sailing?

G: I started to sail about 15 years ago. At that time on smaller lakes and then on bigger and bigger ones and finally across the Atlantic and around Cape Horn.

K: The Atlantic Ocean? Oh!

G: When one has a good boat and if one knowshow to sail in bad weather, it's not much of a problem and it is a great experience. You get away from all the things of the daily life. Secondly, you experience how priorities change. When you are on the land, all these small problems are close to you. When you are out there the priorities change. It's a different world out there.

K: And your brain refreshes.

G: I think that's important as well.

K: Reloaded.

G: Yes.

K: When you face the wide ocean, then you feel you are very tiny.

G: It's beautiful. When you sail across the Atlantic, you sail several days and nights. Before I started sailing on the open ocean, I did some other exciting trips. For example, I crossed Africa with a Jeep from Maroco to South Africa. When I returned from my work in the United States in order to accept a professorship in Germany, I bought myself a car and went from New York to Panama. Shipped the car over to Equador and continued to the very tip of South America. On that trip, I had an opportunity to go with a canoe along one of the tributaries of the Amazon River. This was a lasting experience too.

K: How long usually do you spend sailing? How many days?

G: The longest trip was about three weeks out on the water. That was down from Spain all the way to the Caribic. This trip was part of a Trans-Atlantic race. Another long trip of about three-and-a-half weeks was from the southern tip of South America over the Drake Street to the ice shelf of the Antarctic and back. The distance is not long, but the winds are occasionally very strong there, and the sea may become very rough. Waves with a height of 6 meters are not uncommon. It's quite an experience. If you are in it you ask yourself: why did I do this? However, after the trip one realizes that it is a unique experience.

K: With how many persons?

G: It depends. When I go for smaller sailing trips, I usually go with two friends. One is the former director of a University Hospital, and the other one owns the boat. It's located in a harbor in the Baltic Sea. It is a 42-foot Halberg yacht, a very comfortable boat. There we sail for two weeks or so.

K: Just ten meters long?

G: No. 42 foot is about 13 meters.

K: And for the ocean?

G: For the ocean, in particular when it's rough seas it is comfortable to use a somewhat bigger boat.

K: You used this boat for the Atlantic?

G: No, not this boat. However, a boat of similar size. For the Drake Street we had a boat with a steel hull. The size was about the same.

K: It must be very expensive.

G: Yes, to some extent. The owner of the boat we sail in the Baltic Sea is owned by a former director of a company. He owns the boat and also he takes care of it. That's his hobby. He is an engineer, and for him one part of his sailing hobby is keeping the boat in good condition.

I remember on one of the trips across the Atlantic, we had sometimes storms. So we lost several sails, and in the end we had only one sail left when we came out on the other side. There's not much you can do out on the open water. In particular, you cannot go up the mast because the boat keeps tilting all the time. If a big wave comes, you may fall into the water. In fact, during the Trans-Atlantic race, one skipper tried to repair one of the sails. In order to do so, he was standing at the very front end of the boat. At that moment the wind turned around. The sail turned around as well and threw him into the water. By the time they found him, he was dead. When the waves are high, you can't see a person swimming in the water. Very soon he or she disappears between the waves. On a flat water surface, it would be no problem to pick him/her up. However, if the water is white due to a storm, he/she disappears very fast. So, one has to be careful out there.

Contrary to what many people think, if one is on one of these boats, it's not more dangerous than anywhere else. One is always attached by a rope to the boat. So if something would happen at least one could be pulled back into the boat. In other words, if you don't make a mistake it's not dangerous. Most important is that you have to avoid to panic. That's the most important thing. When you panic, you are in danger. In that sense it is a good training to keep control of yourself.

K: You usually use ropes?

G: Yes, we always have a rope and we use it to attach ourselves to the boat. In fact, one has two ropes. When you walk on the boat, you attach one of the ropes to the boat and detach the other one and then attach this one and so on. So even if something unforeseen happens, you are always attached at least by one rope.

K: So what do your friends in Germany say? Do they think it is dangerous?

G: Yes, occasionally. However, it is not more dangerous than many things in life. For example, crossing a street in a busy city may be more dangerous than sailing, unless you make a mistake.

K: The ratio of dead people by traffic accidents is higher that of sailing.

Okay, thank you very much. I really enjoyed this interview. Thank you again.

Interviewer: Prof. H. Komatsu
in the guest room, WPI Integration Lab. Bldg., September 5th, 2009

Interview with Professor Masaru TSUKADA, Principal Investigator, WPI-AIMR

"Theoretical Research on Surfaces and Interfaces: Past and Present"

--- Open Minds, Originality, and Perseverance ---

Prof. Tsukada (T): I was born in Shanghai on January 1, 1943, in the midst of the Pacific War. In the spring of the year the war ended, I was repatriated to Japan with my mother, my grandmother, and my brothers. I was only three years old and didn't really understand what was happening, but I've been told that my mother and grandmother had a very hard time. My father stayed on at his job and came back to Japan later.

We settled down in Funabashi, in Chiba Prefecture, and I grew up there. Back then, Funabashi was in the country; it seems incredible today, but there were large areas of woods and fields and not many houses. In summer, I ran around in the midst of nature, catching cicadas and grasshoppers. When I reached senior high school, I went to Kaisei Academy a top-ranking private boys' school, whose students in those days went in for a scruffy masculine image, and then I entered the University of Tokyo, in Science Group 1.

The first two years are spent at the Komaba campus, and in the second semester of my sophomore year, professors came from the Faculty of Science on the main Hongo campus to give us lectures. I was particularly impressed by the lectures of Prof. Takahiko Yamanouchi and Prof. Masao Kotani. I was clumsy when it came to hands-on experiments, but I remember being very interested in what Prof. Morizo Hirata had to say.

Prof. Komatsu (K): Prof. Hirata became president of both the Physical Society of Japan and the Japan Society of Applied Physics, and he trained under Torahiko Terada, didn't he? He did pioneering work in unusual fields, such as fracture research.

T: Yes, that's right. Third-year students move to the Hongo campus, and those who intended to do theory had to take an experimental seminar for the first six months. I went to the lab of Prof. Hideji Suzuki, of "dislocation theory" fame, and did tensile tests on single-crystal copper-aluminum alloy. I was there together with Eiichi Kuramoto, who later went to Kyushu University. Toshiyuki Ninomiya, then an assistant professor, was a rising star, and he headed up work on lattice defects. I learned about "dislocation" from these two professors.

In graduate school, my advisor was Prof. Yasutada Uemura, whose specialty was condensed matter theory. A year or two ahead of me in his lab there was a talented lineup that included Kikuo Cho and Eiichi Hanamura. Prof. Hidetoshi Fukuyama was in my year, in the Kubo Lab next door.

Prof. Uemura's approach was to have us discover a topic on our own and develop it freely. He valued the students' own free thinking. There weren't many students then, and there was an atmosphere in which we could take our time and enjoy learning. There were few jobs available that allowed graduates to go on with research, but we all hoped for the best. There was nothing like the post-doc system that exists today, and a lot of people simply stayed on at graduate school as what were called "over-doctors." There were also many people who intended to go overseas and eventually find a job there that way.

For my master's, I tackled the theoretical calculation of electron states in graphite, which Prof. Uemura was interested in at the time. In particular, I investigated the effect of random stacking faults on band structure and calculated their relationship with particular de Haas – van Alphen oscillations. Prof. Uemura was very pleased with this work, and he presented my master's thesis results at an international semiconductor conference. Personally, I developed an interest in such areas as disordered systems, non-crystals, and also surfaces, because I felt that practically everything there was to know about simple, regularly structured materials like crystals was already known, and thus there was no future in that direction.

In the doctoral course, I got interested in various problems of solid-state physics and tackled – to mention just those topics that come to mind – the strongly anisotropic band structure in solids of a one-dimensional nature like tellurium and two-dimensional solids like graphite, and the local electronic states formed by impurities and lattice defects. In the end, I focused on the mechanism that determines electronic states in random alloys. I wanted to establish a principle for calculating the electronic states and phonon spectra, and to create a general theoretical framework. As yet, no effective calculation method existed; all we had was a simple perturbative averaging technique. I wanted to perform electronic state calculations that were expandable and as precise as possible, incorporating the correlation effects of atomic arrangements with a certain degree of precision. After various attempts, I arrived at the approach now known as Molecular Coherent Potential Approximation (Molecular CPA), which has gained international acceptance. This is the most effective way to average randomness, because it doesn't just average, it averages in a way that allows us to incorporate the effects of local structure. At long range, what you have is mostly averaging, but at short range specific differences in atomic configuration can be expressly incorporated. This research was the starting point of my doctoral thesis. When I published it in the *Journal of the Physical Society of Japan* (*JPSJ*), I received reprint requests from many countries. Back before the Internet, we used to request reprints from one another. They poured in from all over the world, and I was happy to know that if one produced good work, it would get a response.

K: This was the paper that marked your international debut, then?

T: This approach was later studied mathematically and became established as the Molecular CPA method. It's clear now that the Green's function has good analytic properties. Some people were trying approaches very like the one I proposed in my paper, and some similar papers appeared after mine. Publishing in a Japanese journal that wasn't yet widely circulated put me at a real disadvantage in terms of name recognition. Authors who published after me but with more fanfare became famous. When it comes to work published long ago, these days people don't seem to care much, doesn't it? Even if one has a greater claim to originality, one is at a disadvantage in terms of name recognition.

T: For my part, I saw that methodology could be fun, and I enjoyed it. I think that was when I discovered the pleasure of developing a methodology that has generality.

As one tries to understand something fundamentally, thinking about methodology opens up new worlds and new concepts. And an approach that has generality can be applied to problems of any kind. This struck me as the essential appeal of physics, and it was very gratifying. So that was my doctoral thesis work.

K: It's not just a matter of understanding, but of equipping oneself with methods for penetrating new territory. That would have been in the 1970s.

T: Right after I obtained my doctorate, I was lucky enough to be made Prof. Uemura's research associate.

K: Who was his assistant professor?

T: Prof. Hiroshi Kamimura. Actually, in Physics Department of the University of Tokyo, on the theoretical side the assistant professors had such an independent status that they held seminars together with the professors. I believe it was different on the experimental side.

At that time, many members of the Uemura Lab were working with two-dimensional electron gas in the surface inversion layer of MOS semiconductors. This has since matured into an important field, following major discoveries like the quantum Hall effect, but in the 1970s the Uemura Lab was the first to undertake theoretical research in this area. On the experimental side, Prof. Shinji Kawaji and his colleagues at Gakushuin University had launched an active research program. In our lab, several years behind me, Tsuneya Ando scored some impressive successes, for example, in the theory of quantum Hall effects in a two-dimensional electron gas and its physical properties.

In my second year as a research associate, I went to do a post-doc under Prof. Wilhelm Brenig, the foremost theoretician in statistical and solid-state physics, at the Technical University of Munich. I was there for two years. This came about when Prof. Ryogo Kubo, who was a friend of Prof. Brenig's, told Prof. Uemura that he was looking for a young researcher. Prof. Brenig was the first person in Europe to deal with the theory of solid-state surface physics and, as it happened, he was about to start work in that field when I went there. I worked on theoretical calculation of the reaction cross section of adsorbed molecules by electron stimulation. The process as a whole is complicated, because the excited state of the adsorbed molecules is immediately de-excited, generating an electron-positive hole pair on the metal side, but I made the calculations using a perturbation expansion of the Dyson diagram. At the Technical University of Munich, there were authorities on the experimental study of electron-stimulated desorption, Prof. Dietrich Menzelproposed MGR theory with Gomer and Redhead, and Prof. Brenig was to provide the theoretical foundation for his experiments.

On my return to Japan in 1974, I wanted to study surface theory, having made a start, but there was hardly anyone in Japan doing theoretical research on surfaces. I happened to be invited to speak at a seminar by Prof. Kenji Tamaru, an authority on catalysts in the Chemistry Department at the University of Tokyo's Faculty of Science, and his lab members showed a lot of interest. That was how I came to get to know people in the chemistry field.

It was a period of truly dramatic advances for "surfaces" as an exact science, marked by the advent of various new experimental measurement methods, such as ultrahigh vacuum techniques. As a nascent field, however, it was still new and unfamiliar to the research community; for example, the Physical Society had no "surfaces and interfaces" category. I recall joining several professors in lobbying the Physical Society to have them recognize a meeting subdivision for "surfaces and interfaces."

K: You are a pioneer of surface science in Japan.

T: After that, I went to the Institute for Molecular Science (IMS) in Okazaki. Hideo Akamatsu was the director at that time. I pursued research there for about five and a half years, in close contact with colleagues in the field known as physical chemistry. This proved very useful in my subsequent research career.

Prof. Keiji Morokuma, a leading young quantum chemist, came back from the United

States to set up a theoretical research arm at IMS after spending two very productive decades at the University of Rochester. Prof. Morokuma had studied under the Nobel laureate Kenichi Fukui, and I took part in the theory group as his associate professor. I met Prof. Morokuma for the first time at IMS, and his energetic style of research had a great influence on me.

K: What was Okazaki like?

T: I'm very fond of Okazaki, I really took a liking to it. We were on the former campus of Aichi University of Education, and it's true that the area wasn't yet developed, so you might be startled by a pheasant flying up when you were strolling along the road. The Institute's driver was a local man, and once he caught a pheasant and we held a barbeque, *yakitori* style.

K: That's hard to believe now.

T: We all lived together in housing for public service employees about ten minutes' walk from the Institute. We were all young, even the professors. There was a lively pioneer spirit in the air.

K: Were you married by then?

T: Yes, I got married shortly before I went to Germany and my wife accompanied me there. She seems to have enjoyed it.

After Okazaki, I returned to the University of Tokyo, Faculty of Science as an associate professor in the Physics Department. At the University of Tokyo, I began to focus on surface and interface theory. At first, I thought about applications of first-principle calculation. I had to make my own density functional method program in the lab. I knew the theory, and based the program on its principles, but it took me two or three years to get the software to work accurately. The grad students in the lab then gradually modified it and created a density functional program package developed entirely in-house. The software is good, it's very reliable. Looking back now, I think we missed a chance: if we'd made the software we developed more user-friendly and released it, it would most likely have been widely used.

By monopolizing the software you've gone to such pains to develop, you can write a lot of papers. In fact, though, you can make a bigger contribution to society by releasing it for others to use all over the world. The only trouble is that if you release it too soon, other people rush to use it and they beat you to the results. It's hard to get the timing or the balance right.

K: At that time, where else in the world was similar research being done?

T: The Fritz Haber Institute in Berlin and UC Berkeley, among others. Students in university labs develop various calculation programs for research use, but when they graduate these tend not to go anywhere. I approve of students' developing software if it's an integral part of the science, but I wouldn't want to make it an end in itself, and so perhaps it's inevitable. If software development becomes an end in itself, I don't think we can call that true academic work.

Today, commercial software is readily available and you don't even need experience to use it. But problems arise when the software becomes a "black box": the user can't judge whether the results are correct. The data may have been inputted wrongly and nobody noticed. Ideally, the user should have a good knowledge of what happens inside the black box and of the physical phenomenon being studied.

K: The drawback in using a "black box" is that it doesn't lead anywhere new. One can't locate the problems in terms of the limits of application, accuracy, and so on.

T: In surface research, I also took a look at the atomic arrangements in reconstructed surfaces of silicon and other semiconductor crystals, which were hot topics at the time – such things as the structure of Si (111)-7×7 surfaces. Experimentally, dozens of structural models had been put forward, but I gradually came to favor the DAS model proposed by Prof. Kunio Takayanagi of Tokyo Institute of Technology. What finally decided the question, of course, was the scanning tunneling microscope (STM).

The structure and kinetics of Si (100) surfaces were another major area of surface research where experiments and theory combined to give results. The atomic reconstruction differs for each low-temperature region. It isn't simple, because STM observations show that the true structure is influenced by electron excitation due to electron injection. Moreover, atomic force microscopy shows a different structure from that given by STM. Recently, however, this problem has been settled, up to a point.

I worked jointly with Masakazu Aono of the National Institute for Research in Inorganic Materials (now part of the National Institute for Materials Science) on an interesting problem relating to low- energy ion scattering spectroscopy. When you direct helium atoms at the specimen surface, you get two peaks in the energy spectrum of the reflected ions. We found that this was due to a process in which the incident helium ions are first neutralized and then re-ionized. We were delighted when, using a simple theoretical analysis, we succeeded in explaining this fully in terms of a kinetic process involving movement of both electron and ion, but it is also a kind of observational problem.

Another interesting research subject was elementary processes in field evaporation. We set out to theoretically elucidate the mechanism that causes atoms to evaporate one by one when a strong positive potential is applied to a needle specimen. It's an extremely interesting question, as the mechanism involves competition between adiabatic and non-adiabatic effects. We traced the transitions theoretically in great detail. We were personally satisfied with our careful analysis, but if one gets too abstruse, it doesn't go over well, right?

Lately, I've become interested in the electrochemical aspects of the field. For example, redox reactions at electrode surfaces: these are chemical reaction processes occurring in solution, triggered by electron transfer. Field evaporation is traditionally a phenomenon that occurs at metal surfaces under ultra-high vacuum, but, in a certain sense, the phenomena at interfaces in aqueous solution can be said to resemble field evaporation, to be an extension of the same principle. I want to make this one of the central topics in my laboratory at WPI-AIMR. At the same time, I want to work toward making theoretical connections with the atomic-level structure, kinetic changes, reactions induced by electron transfer, and other observations that can be made by STM and atomic force microscopy (AFM) at the electrode-solution interface.

Theoretical research relating to STM and AFM has also ended up as part of my life's work. When these experimental techniques were first invented, it was a mystery to me how atoms could be imaged with an STM probe whose radius of curvature is on the order of 10 nm. By doing electronic state calculations for both the probe and the sample surface and using them to calculate the tunnel current, we succeeded in reproducing atomic-scale images like those obtained experimentally. We were also able to show how the atomic-scale images are influenced by the shape and structure of the probe.

K: Does that mean that the tip of the probe is not spherical, but consists of a single atom?

T: That's correct. It means that the tunnel current and the atomic forces are concentrated almost in a single atom at the very tip. In the theory of STM, the tip of the probe had previously been assumed to have perfect spherical symmetry and the effects of probe structure had not been taken sufficiently into account. When two or more atoms interact with the tunnel current, they interfere with each other and you can't obtain a clear image. But with a single atom at the needle tip, the image has excellent atomic resolution.

K: Can't these results be utilized in experimental measurements?

T: Many STM and AFM images cannot be understood in solely experimental terms, but theoretical calculations make it possible to interpret them correctly, and in some cases to analyze them quantitatively. Further, theory allows us to predict new functions of scanning probe microscopy (SPM) and suggest these to the experimental people. SPM has made striking progress recently in a wide range of fields, including biotechnology; it is even beginning to rival various spectroscopy methods, including nonlinear effects in optical, infrared, and ultraviolet spectroscopy. SPM theory is taking on an ever-greater role in support of such developments.

In addition, it has recently become possible to identify and manipulate atoms by AFM. In experiments of this kind, the minute details of the shape of the probe tip have an impact. The atomic forces are fundamental in these cases, rather than the tunnel current….

K: What exactly are the atomic forces?

T: At long range, you have van der Waals forces, and then there is also a kind of electrostatic force. As the probe's proximity to the sample increases, a force known as chemical interaction force is generated by quantum hybridization effects of the electron wave function. At still closer proximity, there occurs a strong repulsive force that stems from the effect of the Pauli exclusion principle. In an atomic force microscope, measurements are performed in the range where the attractive force is gradually increasing. The situation is complicated by the fact that, while the probe as a whole is subject to attractive force, repulsive force is beginning to act at its tip. This fact becomes relevant to the mechanism of atom manipulation.

Friction force microscopy has also yielded some very interesting findings. According to experiments that used an AFM probe to investigate friction at the atomic level, forces are generated parallel and perpendicular to the direction in which the probe is scanned. This situation can be reproduced beautifully by theoretical simulation. The results of such simulations have shown that friction force microscope images like these are formed by atomic-level stick-slip.

K: So when you can do a theoretical simulation of results obtained experimentally, you're convinced? Can you turn that around and predict experimental results?

T: Yes, of course. For example, we have predicted theoretically that when a coherent current flows through a large molecule or through graphene, the internal current will show a strong loop current feature, but this doesn't seem to have been confirmed experimentally as yet. With regard to SPM simulation, I am presently attempting to solve the so-called "reverse problem," that is, to use measurements of standard samples or target samples to determine the probe structure and sample structure. In another role for SPM simulation, we sometimes correctly interpret and quantitatively analyze images that cannot be understood on a purely experimental basis. For instance, with AFM experimental data from samples in solution, it is often quite impossible to draw an intuitive picture. In such cases, theoretical simulation brings great power into play.

K: I've heard it said that real theoreticians don't use computers? It's also said that people turn things over to a computer because they're stuck.

T: Some people might say that, yes.

In research, lately I've come to realize that finding the way out is important. With regard to SPM theory, I'm currently involved in a JST program of "Development of System and Technology for Advanced Measurement and Analysis." The SPM simulation project calls for building, demonstrating, and commercializing a prototype simulator.

K: I guess that's what's wanted in these times? You're certainly involved in a lot of projects.

T: Well, in fact, that's a rather difficult question. In fact, I think that when one becomes involved in such work, one tends to lose a little of the true joy of doing science, but I suppose it's important from a social standpoint.

K: I know what you mean. It's the murky areas that interest you, and once they're cleared up, you lose the intense determination that was driving you. That I can understand very well. The same thing happens with experiments.

T: In the style of research I used to pursue, I would stop once I had an idea of how things were going to turn out. Actually, though, it seems to me that there are things that everyone thinks they already know when in fact they don't, and that sometimes openings like that can lead to some very innovative science.

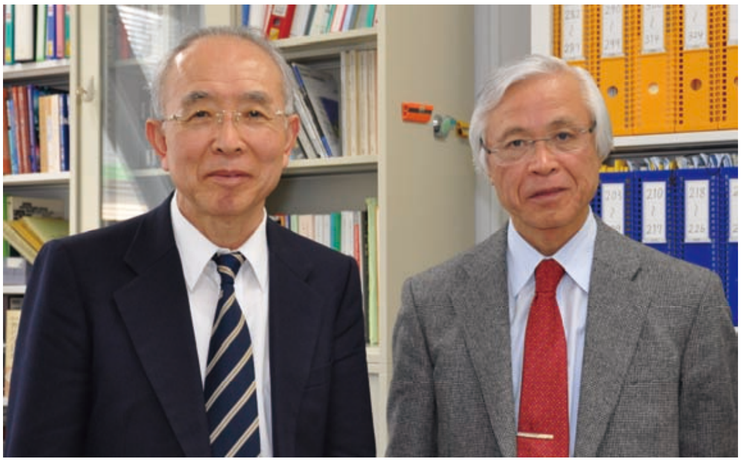
K: It's like the "black box" we were speaking of earlier. It's taken for granted and one doesn't even think about what's inside.

T: In that connection, you might be wondering why I study organic thin films when they've already been commercialized, but we still don't know a lot of fundamental things regarding their electronic states and electron mobility. For example, at the most fundamental level of all, there's the molecule-electrode link structure at the interface and the related physics. To make it possible to move ahead and take the step of developing revolutionary, I want to clarify the basics, centered on molecular bridges, and to understand them properly at the atomic level. I also want to explore the unexpected quantum functions of molecules and make proposals to experimental researchers accordingly.

K: In that sense, am I right in thinking that here at WPI, you have the chance to gain the maximum advantage from all the research that you have built up over the years?

T: Yes, there are a lot of research topics likely to yield interesting discoveries if we work on them here together.

K: I don't want to sound like I'm bragging, but there's Prof. Kingo Itaya's liquid STM



work, and Prof. Kawasaki's experiments on oxides, shear bands in BMG, to name just a few. There's a natural fusion, isn't there?

T: We don't have time to go into detail now, but I'd also like to do various studies from a theoretical viewpoint on BMG.

K: Would you like to tell us about your policy in your research, or what advice you give your students?

T: It may sound trite, but I think doing science comes down to simple curiosity, and the enthusiasm and originality to find out the answers. You can't do anything if you just follow others. I'd say you need to be strongly motivated as an individual, and in real earnest.

K: Dr. Bednorz of IBM talked about that in a recent interview. It's like what he said about not being carried along with everyone else, even swimming against the current if you have to.

T: I'm very happy to have been invited to WPI.

K: WPI is very lucky to have a theoretician like yourself, Professor. This is a key laboratory for fusion. I want to ask leading theoreticians from around the world to come here, even if only for a short time, because we have few restrictions in that regard.

Lastly, could you give a word of advice to those who are about to embark on their careers?

T: A number of things are important. One is to maintain a sustained interest. Perseverance is might. But I don't mean you should persevere in a narrow field and with a fixed methodology. I mean you should discover big questions that you want to solve yourself among natural phenomena or science and technology, valuing your own ability to keep an open mind, and then persevere in studying those questions from every angle, in an interdisciplinary way, until you arrive at the solution.

K: In the end, people do what they enjoy, don't they?

T: If you do something because you're forced to, you won't keep it up. Nothing will come of it unless you think for yourself, freely and essentially.

K: The spirit of adventure is gradually dying out, isn't it? Who is the researcher you respect the most?

T: Lev Davidovich Landau. Though I couldn't be like him if I tried, he was a great man. He had a clear way of thinking. He gets to the essence of things in simple language.

K: This has been a most enlightening discussion. We haven't talked much about failures, but I think there's probably a mass of them behind any successful piece of research. Thank you.

Interviewer: Prof. H. Komatsu
in Prof. Tsukada's office in the WPI-AIMR Annex, April 21st*, 2009*

WPI-AIMR PI　塚田捷教授にきく
(Interview with Professor Masaru TSUKADA－Japanese version)

表面・界面の理論研究の今昔

---自由な発想と独創、そして持続---

塚田：私は昭和 18 年 1 月 1 日に上海で生れました。太平洋戦争の最中です。終戦の年の春に母や祖母、兄弟たちと一緒に引き上げてきました。3 歳の時ですから、私にはよくわかりませんでしたが、母や祖母は大変苦労をしたそうです。父は外地の勤め先に留まっていて、後から帰国しました。

私たちは千葉県の船橋に落ち着き、その後ずっとそこで育ちました。当時の船橋は今では考えられないくらい田舎で、人家も少なく、雑木林や畑が広々としていました。夏は蝉やバッタを自然の中で追いまわしました。高校は当時はばんからだった開成にゆき、東大の理科一類に入学しました。

2 年生の後半には本郷から理学部の先生の講義がありました。中でも素粒子の山内恭彦先生、物性の小谷正雄先生の講義には感銘を受けました。私は実験で直接手を動かすことでは不器用でしたが、平田森三先生のお話は大変面白かったことを記憶しています。

小松：平田先生は物理学会、応用物理学会ともに会長をなさった方で寺田寅彦のお弟子さんですね。割れ目の研究などユニークな分野を開拓されました。

塚田：そうです。3 年生になって本郷に行くのですが、理論志望の学生は半年間、実験の研究室で勉強することになっていました。私は「転位論」の鈴木秀次先生のところにゆき、銅単結晶の引張り試験をしました。九大に行った蔵本英一さんも一緒でした。二宮敏行先生は新進気鋭の助教授で、「格子欠陥」の旗頭でした。このお二人から「転位」のことを学びました。

大学院は「固体電子論」の植村泰忠先生の所に行きました。研究室の数年上の先輩には張紀久夫さん、花村榮一さんなど多彩な方々がいます。久保研に行った福山秀敏さんは、隣の久保研究室で同級生です。

植村先生の方針は、自由に自分でテーマを見つけて展開せよということで、学生自身の自由な発想をとても大切にされていました。当時は学生数も少なく、ゆっくりと学問を楽しむことのできる雰囲気がありました。研究が続けられるような就職口は少なかったのですが、なんとかなるさと皆が楽観的でした。今のポスドクのような制度もなく、そのまま大学院に残るオーバードクターが大勢いました。外国に出てそのうち何とか職を見つけようなどという人たちも多かったのです。

修士課程では当時植村先生が興味を持っておられたグラファイトの電子状態の理論計算に取り組みました。特にランダムに入った積層欠陥がバンド構造に及ぼす影響を調べ、特

殊なドハースファンアルフェン振動との関係などを計算しました。植村先生は大変喜んでくださって、修士論文の成果を半導体国際会議で紹介して下さいました。私自身は、結晶のように構造がきちんとした単純な物質はもう殆どが分かっていて、先がないような気がしていたものですから、乱れた系、結晶でないもの、表面もそうですが、そんなところに興味を感じていました。

博士コースに入ってからは物性物理のいろいろな問題に興味を持ちましたが、記憶に残っているものとしては、異方性の強いたとえばテルルのような一次元的な固体や、グラファイトのような二次元性固体などのバンド構造や、不純物や格子欠陥が形成する局所的な電子状態などに取り組みました。最終的にはランダム系の合金で、その電子状態がどのような機構で決まるのかに興味を持ちました。電子状態やフォノンスペクトラムを計算するための原理を明らかにして、一般的な理論のフレイムワークを作りたいと思った訳です。それまでは有効な計算方法ができておらず、摂動的に平均化をする素朴な方法があっただけです。原子配列の相関効果をある程度正確に取り入れ、できるだけ正確で発展性のある電子状態の計算をしたいと考えていました。いろいろな試みをした結果、一つの考えに到達しました。今では分子CPA（Molecular Coherent Potential Approximation）と呼ばれて国際的に通っていますが、これはランダムネスを最も有効に平均化する方法です。単に平均化するのではなく、局所構造の効果を取り入れることができるように平均化します。遠いところは殆ど平均化されるが、近くでは個々の原子の配置の違いがあらわに取り入れられるという方法です。この研究が博士論文の出発点になりました。JPSJ（Journal of the Physical Society of Japan）に出したら、各国から別刷り請求が多数来ました。インターネットが無かった当時では別刷り請求を互いによくしたものでした。ずいぶんたくさんの請求が世界各国から来て、良いものを出せば反響があることがわかり大変嬉しかったです。

小松：先生の国際的な最初のデビュー作ですね。

塚田：その後、この考え方は数学的にも検討され MolecularCPA 法として確立され、グリーン関数が解析的に良い性質をもつことが明確になっています。私が発表した提案に大変近い方法で試みをしていた人たちや、私の後にやった人たちがいました。私はサーキュレーションがまだよくなかった日本のジャーナルに出したものですから、知名度という点ではずいぶん損をしました。後から派手にアピールしたほうが有名になったのです。最近の人は昔の仕事は誰がやっていようと、どうでもよいというところがありますね。

小松：これは日本人にはよくあることですね。オリジナリティーはこちらにあっても、知名度で損をする。

塚田：私自身は方法論の面白さに気づき、楽しかったです。一般性のある方法論を作り上げる楽しさをこれで覚えた気がします。

ものごとを根本から理解しようとしているうちに、方法論の検討から新しい世界や新しいコンセプトが開けてくるし、一般性があればどんな問題にでも使える、ここが物理学のだいご味のような感じがして嬉しかったです。これが博士論文の仕事です。

小松：単に理解するだけでなく、新しい領域に攻め込んでゆく方法を身に付けることにもなりますね。これが 1970 年代ですね。

塚田：博士を得た直後、大変ラッキーなことに、植村先生の助手にしてもらいました。

小松：助教授の方はどなたでしたか。

塚田：上村洸先生でした。もっとも東大の物理教室では、理論系の研究室は助教授の人たちも独立していて、教授の研究室とはセミナーを一緒にやるくらいでした。実験系はそうではなかったようですが。

その当時、植村研の多くの方が、MOS 半導体表面反転層における二次元系電子ガスを扱っていました。今では量子ホール効果などという大発見もあり大分野として成熟していますが、1970 年代の当時、植村研が初めて理論面の研究に着手したものです。実験面は学習院大学の川路紳治先生たちが活発な研究を始めていました。研究室の私の数年後輩に安藤恒也さんがいましたが、二次元電子ガスの磁気抵抗効果やその物性に関する理論などで素晴らしい成功を収めていました。

私は助手になって 2 年目に、統計物理理論や固体理論の大御所であるミュンヘン工科大学のウィルヘルム・ブレニッヒ先生の所にポスドクで行き、2 年間滞在しました。久保亮五先生と親しかったブレニッヒ教授が若い研究者を探していると、植村先生に話されたのがきっかけです。ブレニッヒ教授は固体表面物理の理論をヨーロッパで最初に手掛けた人です。私は、同教授がその分野を丁度スタートさせる時期に行ったことになります。表面上の吸着分子が電子刺激で脱離するときの反応断面積を理論的に計算する仕事をしました。吸着結合の励起状態は金属側の電子正孔対を生成してすぐさま脱励起するので、全体のプロセスは複雑になりますが、それをダイソンダイアグラムの摂動展開で計算しました。ミュンヘン工科大学には、メンツェル教授という電子刺激脱離の実験の大家がいましたが、この実験の理論的基礎をブレニッヒ先生が与えることになりました。

1974 年に帰国したとき、せっかく勉強しはじめたということもあり表面の理論を志していたのですが、日本には表面の理論研究者は殆どいませんでした。たまたま東大理学部の化学教室に触媒研究の大家である田丸謙二先生がいて、研究室セミナーに呼ばれて話に行きましたが、そのとき研究室の方々から大変に興味を持ってもらいました。そこで化学の方々と知り合うきっかけになりました。

当時は精密科学としての「表面」は超高真空技術をはじめ新しい計測実験手法がいろいろと生れ、まさに勃興期でした。しかし、新しく誕生した分野なので、多くの研究者にとってなじみのない新しい分野であり、例えば物理学会には「表面・界面」などという分野もなかったのです。　物理学会に「表面・界面」の分科を認めてもらうように、何人かの先生方と運動したことを記憶しております。

小松：表面科学の草分けですね。

塚田：その後、岡崎の分子科学研究所（分子研）にゆきました。赤松秀雄所長時代です。そこで約 5 年半研究生活を送りましたが、物理化学と呼ばれる分野の方々と親しく交流す

ることができ、私のその後の研究歴にとって非常に有益でした。

量子化学分野の若手の大家であった諸熊教授が、二十数年間ロチェスター大学で活躍された後、分子研の理論研究系を創設するために米国から帰ってこられました。諸熊先生はノーベル賞の福井謙一先生のお弟子さんですが、私は諸熊教授の助教綬として理論グループに参加しました。私はこの諸熊教授と分子研で初めてお会いして、そのエネルギッシュな研究ぶりを拝見して大きな影響をうけました。

小松：岡崎はどうでしたか？

塚田：私は大変岡崎が好きで、気に入っていました。たしか愛知教育大学の移転跡で、当時は付近の開発が進んでいなくて、何げなく道を歩いているとキジが飛び出てきたりしました。運転手さんが土地の人で、そのキジを捕えて焼き鳥パーティーをしたこともありました（大笑い)。

小松：今では信じられませんね。

塚田：研究所から歩いて 10 分くらいのところが公務員宿舎で、皆、一緒に住んでいました。教授の方々を含め、皆若かったですね。草創期の活気にあふれていました。

小松：先生はご結婚されていたのですか？

塚田：はい、ドイツに行く少し前に結婚していて、二人でドイツに滞在しました。家内は楽しかったようです。

岡崎のあと、東大理学部の物理教室へ助教授になって戻りました。東大では表面・界面の理論を中心に研究を始めました。最初に第一原理計算の適用を考えました。密度汎関数法による計算法のプログラム自体を、研究室で自作せねばなりませんでした。理論そのものはわかっているので、その原理をもとに作るのですが、正確に動くソフトにするためには 2、3 年かかりました。その後も研究室の院生が少しずつ手を加えていって、自前の密度汎関数用のプログラムパッケージを作りました。このソフトウエアは非常に信頼度の高く良いものです。今になって考えると、ここで開拓したソフトをもっと使い易くして一般に公開すれば、広く定着したのではないかと残念に思います。

自分が苦心して作ったソフトで、独占してやればどんどん論文が書けます。しかし、本当はこれを世界中に公開して皆が使えるようにした方が、世の中の役に立って貢献ができるということです。ただ公開が早すぎると他でどんどん使われて、成果を取られてしまう。その公開のタイミングやバランスがむつかしいです。

小松：当時、世界ではどのあたりが先生の研究に近い研究をしていましたか？

塚田：ベルリンのフリッツ・ハーバー研究所やカリフォルニア・バークレイ校などです。大学の研究室では学生がいろいろ研究用の計算プログラムを作っていますが、卒業すると立消えになることが多いのです。ソフトはサイエンスの一環として学生が作るのは良いのですが、学生をそれだけに使ってしまうことはしたくないのでやむをえないこともあります。ソフトつくりそのものが目的になるようになったら、学問とは言えないと思います。

今ではコマーシャルベースでソフトが自由に手に入り、経験のない人も使えます。ただ

その時に問題なのは、ソフトが「ブラックボックス」となった場合です。結果が正しいかどうか判断できません。入力が間違っていても気づかないことも出てきます。ブラックボックス内の仕組みや、対象の物理現象がよく分かっている人が使う分にはよいのですが。

小松：「ブラックボックス」を使うことの欠点は、そこから新しい発展が生れない。適用限界や精度のどこに問題があるのか判断できない。

塚田：表面の研究では、当時ホットな話題だったシリコン、その他の半導体結晶表面の再構成原子配列、例のSi（111）面の7×7構造なども手がけました。実験的には何十という構造モデルが提案されたのですが、東工大の高柳教授のDASモデルが良いらしいということが、段々に分かって来ました。しかし最後の決め手はSTM（走査トンネル顕微鏡）でしたね。

また、シリコンの（100）面の構造や動的過程などが、実験と理論とが協力して成果を生んだ表面研究の大きな流れでした。低温での温度領域ごとに原子再構成の様子が変わります。STMによる観測では、電子注入による電子励起によって真の構造が影響を受けるので単純ではないのです。また、原子間力顕微鏡ではSTMによるものとは異なる構造が見出されます。しかし、最近ではある程度、この問題に決着がついてきました。

低速イオン散乱分光に関連して、無機材研（現、物質材料研究機構）の青野正和さんと共同研究した問題も面白かったです。試料表面にヘリウム原子を当てると反射イオンのエネルギースペクトルにピークが2つ出るのですが、それは入射ヘリウムイオンがいったん中性化されてから再イオン化するプロセスが含まれるためであることが分かりました。電子移動とイオンの運動とが絡み合った動的過程として、簡単な理論解析ですべて説明できたときは嬉しかったですが、これは一種の観測問題にもなっているのです。

電界蒸発の素過程の研究も、興味あるものでした。試料を針状にして強い正電位を与え、原子を一つずつ蒸発させるメカニズムの理論的解明です。そのメカニズムには断熱性と非断熱性の競合がありとても面白い問題なのですが、その移り変わりを丁寧に理論的に解明しました。私たちはきちんと解析して満足したのですが、あまりむつかしいことをいっても受けませんね（笑い）。

ところがここ最近になりまして電気化学系、例えば、電極表面における酸化還元反応に興味を持つようになりました。電子移動がトリガーする溶液内の化学反応過程です。電界蒸発は超高真空下での金属表面上の現象でしたが、今度は水溶液内の界面上の現象で、ある意味では電界蒸発と類似したその発展的な現象といえます。WPI-AIMRでの私の研究室の中心テーマの一つにしたいと思っています。一方、STMやAFM（原子間力顕微鏡）で観察される電極・溶液界面上の原子レベル構造、動的変化、それと電子移動が誘起する反応などの理論とも関連させて研究を進めたいと思っています。

走査トンネル顕微鏡（STM）や原子間力顕微鏡（AFM）の理論研究も、私のライフワークの一環となってしまいました。これらの実験法が発明された当初は、なぜ曲率半径が10nm程もある探針でSTM像として原子が見えるのか？全く分からなかったのです。私た

ちは、探針と試料表面の双方で電子状態計算を計算し、これからトンネル電流を計算することにより、実験で観察されるような原子尺度イメージを再現することに成功しました。探針の形状や構造がどのように原子尺度像に影響するかも明らかに出来ました。

小松：プローブの先端は球状でなく、1原子ということですか。

塚田：そうです。最先端の 1 原子にトンネル電流や原子間力が集中しているということです。それまでSTMの理論では、プローブの先端を完全な球対称に仮定して針の構造の効果をきちんと考えていなかったのです。2つ以上の原子がトンネル電流に関連してくると、互いに干渉しあってきれいな像が得られなくなりますが、針先端に一個だけ原子がある場合には像が見事に原子分解能を示すようになります。

小松：この結果は実験の計測に活用できませんか？

塚田：実験だけからでは理解できないSTM像やAFM像は多いのですが、理論計算によりこれらを正確に解釈し、場合によっては定量的に解析することが可能となります。さらに走査型プローブ顕微鏡（SPM）の新しい機能を理論的に予測し、実験家に提言することもできます。最近の SPM の進歩は、バイオ系を含め広汎な分野で目覚ましく、可視、赤外、紫外の非線形効果を含めたさまざまな分光法にも匹敵するようになりつつありますが、そのようなSPMの展開を可能とするためにSPM理論の役割はますます大きくなっています。

また、AFMで原子の同定や原子を動かす操作をすることが、最近では可能となっています。このような実験になると、針先端の詳細な形状が影響するようになります。この場合はトンネル電流でなく原子間力が本質的ですが…。

小松：ところで原子間力の実体は何ですか？

塚田：遠方ではファンデルワールス力で、イオン化していれば静電気力的なものも入りますが、探針と試料とが近接するにつれて、化学的相互作用力といって波動関数の量子的混成効果によって力が発生します。もっと接近するとパウリの排他律に起因する強い反発力が生じます。原子間力顕微鏡では、引力が少しずつ強まる領域で計測しています。複雑なのは針全体としては引力を感じますが、先端部分は斥力が働き始めていることです。このことはアトム・マニピュレイションのメカニズムに絡んできます。

摩擦力顕微鏡にも興味深い発見があります。AFM探針で原子レベルの摩擦を調べた実験によりますと、針を引張る方向と直角の方向に力が発生したりします。このような状況を理論シミュレーションは、見事に再現することができます。原子レベルのステック・スリップにより、このような摩擦力顕微鏡像が形成されることを、理論シミュレーションの結果は示しました。

小松：実験で得られたことを理論的にシミュレーションして納得するのですか。逆にプレディクション（予想）もできますか？

塚田：これはもちろん可能です。例えば大きな分子やグラフェン内部にコヒーレントな電流が流れるときの内部電流に、強いループ電流が流れることを理論的に予言していますが、まだ確認できるような実験はできていないようです。SPMのシミュレーションに関しては、

標準試料や対象試料の計測結果から探針構造と試料構造とを決定する、いわゆる逆問題を解きたいと思いまして今試みています。また、SPM シミュレーションの役割としては、実験だけでは全く理解できない像の正しい解釈と定量的な解析をすることもあります。例えば、溶液中試料の原子間力顕微鏡の実験データは、直観的な猫像が全く描けないものが多いのです。このような場合に、理論シミュレーションは大きな威力を発揮します。

小松：まっとうな理論家はコンピュータを使わないなどといいますが？出来ないからコンピュータに持ち込むなどという人もいますが。

塚田：そういう人もいるかもしれません（笑い）。

研究には出口が大切なことも、最近、認識するようになりました。SPM 理論に関連して、現在 JST（独立法人科学技術振興機構）の先端計測プロジェクトに参加しています。プロトタイプのシミュレータを作成して、これを実証実用化する計画です。

小松：時代の要求ですか。仕事が一杯ですね。

塚田：いや、本当はそこのところが少し難しいのです。そのようなところでサイエンスの醍醐味が少し失われるようにも思いますが、社会的な見地からは重要ではないでしょうか。

小松：そうですね。混沌としたところにこそ面白みがあり、判ってきたらもうやるファイトを失うということ、よく分かります。実験も同じことがあります。

塚田：従来の私の研究の流儀では、見当がついてくると止めていました。しかし、その逆に、皆が分かっていると思っていることの中に、実は本当のところが分かっていないこともあり、そこからまた非常に革新的な科学が開けるということもありうるのではないでしょうか？

小松：先ほどの「ブラックボックス」ですね。もう決まり切ったもので内容を検討することもしない。

塚田：その点で有機薄膜はもう実用化されているのに何でやるのといわれるかもしれませんが、電子状態や電子移動に関連して、基本的なところがよくわかっていないことが多いのです。例えば、もっとも本質的な界面での電極と分子とのリンク構造とこれに関係する電子物性や電子移動のメカニズムです。現状を超えて次世代の画期的な機能系を開発するステップを可能とするため、分子架橋系を中心に、基本的なことを原子レベルで解明しきちんと理解しておきたいと思っています。同時に分子の思いがけない量子的な機能を探索し実験家に提言したいと思います。

小松：そういう意味ではこれまで先生が積み重ねてこられた研究がこの WPI で活かせるチャンスですね。

塚田：ここには一緒にやったら面白いことが分りそうだという研究がいっぱいあります。

小松：私が言うのは変ですが、板谷先生の液中STMや、川崎先生の実験、BMG の Shear band など、いろいろありそうですね。自然にフュージョン（Fusion）しますね。

塚田：詳しくお話しする時間ももうありませんが、BMG も理論の立場からいろいろと研究したいですね。

小松：先生の研究上のポリシーや学生さんによく言っていることを教えて下さいませんか？

塚田：月並みですが、サイエンスは素朴な好奇心と、これを解明しようとする熱意と独創性に尽きると思います。人の後追いでは何もやれない。個人がハングリーで真剣勝負をすることでしょうか。

小松：それはこの前のインタビューでも IBM のベドノルツさんが言っていましたが、「人と同じ流れに乗らない。場合によっては流れに逆行する」と同じですね。

塚田：私は WPI に来させていただいてすごく幸せです。

小松：いや、WPI も先生のような理論家がいることが幸せです。フュージョンのキイラボラトリーです。世界中から優秀な理論家に短期間でもいいから来ていただくこともお願いしたいです。WPI は人に来ていただく上での制限が少ないはずですから。

最後に、これから伸びてゆこうとする人たちに一言お願いします。

塚田：いろいろありますね。一つは持続した興味を持つこと。「持続は力なり」ですね。ただし、これは限定した分野でしかも決まった方法論で研究を続けるという意味では全くありません。自分の素朴な発想を大事にしながら、自然現象や科学技術の中で、自ら解き明かしたい大きな問題を発見すること、その解決にせまるために分野を超えてあらゆる角度から研究を続けるということです。

小松：人は結局は好きなことをやっていますね。

塚田：人に強制されてすることは続きませんね。自由に実質的に自分で考えてすることがないと何も生れませんね。

小松：冒険心が段々小さくなってきていますね。尊敬する研究者どんな人ですか？

塚田：ランダウ（Lev Davidovich Landau）ですね。彼のように成りたくてもなれませんが、すごい人ですね。考え方がクリヤーですので。簡単な表現で本質をつきますね。

小松：今日は大変勉強になりました。失敗の話は余りありませんでしたが、多分一つの研究の裏には失敗の山積みがあると思います。ありがとうございました。

2009年4月21日
WPI-AIMR アネックス棟　PI 塚田捷教授研究室にて
小松　啓（ひろし）

Interview with Professor John H. PEREPEZKO, Professor, University of Wisconsin-Madison & Adjunct Professor, WPI-AIMR

“We must have a long view of science”

---You cannot shorten time with extra money---

Prof. Perepezko (P): I grew up in New York City and then when I was a teenager I moved to a suburb called Long Island.

Prof. Komatsu (K): Long Island, I see. Beautiful place, maybe.

P: That is where I went to high school. Yes, it was a really good environment at that time. I did my undergraduate work at the Polytechnic Institute of Brooklyn. The name has changed a few times and it is now merged with New York University. There, I studied metallurgical engineering. I was always interested in making things and working with different types of materials. It was really fascinating to study formally different materials and to work on laboratory experiments.

I remember once my father gave me some materials and said that if you are a good materials person, tell me what these are. I had only a few tools at home, but I was able to determine that they were actually semiconductors and he was very impressed.

K: It was right.

P: Yes, it turned out to be correct. After I finished my Masters program I went to Pittsburgh and I worked for 2 years at the United States Steel Research Laboratory. This was a very famous place at that time.

K: Yeah, U.S. Steel is a big company internationally known.

P: Right. The head of the laboratory was L. S. Darken.

K: Famous book “Physical Chemistry of Metals” was written by Darken and Gurry.

P: Darken and Gurry, yes. I was the youngest member and at lunch table were all these famous people who published in the journals that I read.

K: Very good.

P: In fact, the group I was working in had the first Field Ion Microscope, atom probe machines. This was in 1969. The man who made it was Sid Brenner. I went to graduate school in the evening at Carnegie Mellon University and worked during the day. After leaving U.S. Steel, I was able to finish my PhD degree full time. My advisor was Professor Massalski.

K: T. B. Massalski is a famous teacher. “Structure of Metals” by Barret and Massalski is well known.

P: I was able to continue my interest in materials with him and work on phase transformations. During that time I became very interested in nucleation reactions and that continues today. As you know, all transformations have to start somewhere and nucleation is an important aspect, including bulk metallic glasses where the objective is to avoid nucleation. In order to control a transformation process you must understand the mechanism.

K: You have been to Stanford?

P: No.

K: I thought you might have been in Stanford where you met Prof. Kazumi Nishioka since he got Ph.D. at Stanford and I often heard your name from him. Then where did you meet him?

P: I met him because he came to Michigan Technological University for a sabbatical and he visited me in Madison. I had one of his students as a Ph.D. student in my laboratory. That is how we made contact. We had some exchanges after this but his department was precision mechanics and our communication decreased over time.

K: Yes, he graduated at Osaka University originally, and he got a position in Tokushima University. Have you been to Tokushima?

P: No, I have not.

K: You have not been there?

P: No. I have visited many places in Japan but not Tokushima. Anyhow, nucleation has been one of my main interests and also it relates to phase stability which is another important part of bulk metallic glasses. You know famous three golden rules of Professor Inoue are all related to phase stability.

K: Yes. So, your father was also an engineer?

P: No.

K: Because he put semiconductor to you.

P: Right. But he worked in the construction business. He would come to different places and one time he was at a semiconductor plant.

K: That is why he had semiconductor.

P: Right. He did not tell me that though.

K: I see, very interesting.

P: Yes, now I have been in Madison for over 30 years at the University of Wisconsin and it is a very nice town to live in. My children have grown up there and they have enjoyed it very much. I have been able to work with many very bright students and see them develop their careers afterwards. It is very nice.

K: Yes, and maybe next topics.

P: Motivation to science.

K: Yes, when it started?

P: When it started? I think as a small child I was always curious about things and I built a little crystal radio.

K: That was about 1950?

P: Ye, you could build things like that in those days, simple things. I remember I made some castings from lead alloys on the kitchen stove. I was also interested in alloys. Materials was something I enjoyed. I remember being fascinated to watch a blacksmith once as a child and how he made this iron pieces.

K: Naturally, you developed taste for industries; mechanical or material science gradually and you selected university in that sense.

P: Exactly.

K: Brooklyn Polytechnic Institute.

P: Right. And when I went to Pittsburgh, Carnegie Mellon University was the top school and had a long history.

K: So you did some work in the Carnegie Mellon? What sort of work did you do?

P: My thesis work was on phase transformations, a solid-state transformation called the massive transformation.

K: And your professor was Massalski.

P: He was very famous in that area. I was growing single crystals using solid state phase transformation and I measured the kinetics of transformation.

K: What sort of material did you use?

P: I worked on iron- nickel alloys and also silver-aluminum alloys. I stayed a short time after my Ph.D. to do some postdoctoral work and then I got a call at Wisconsin. At Wisconsin I started my work on solidification because during the time I was at Carnegie Mellon, there were other graduate students studying rapid solidification. I found rapid solidification to be interesting and started to work on that at Wisconsin.

K: I see. Around what time of the year?

P: This is 1975. Then, while at Wisconsin I worked with some colleagues and we developed droplet techniques for getting very large liquid undercooling to study formation of metastable phases and amorphous phases. We made careful measurements of some of the properties such as specific heat and analyzed the different phases that are produced during solidification because these different phases have different structures and different properties. This was in the early 1980s.

K: Did you do laser fusion?

P: No, we studies liquid droplets that showed a large undercooling during slow cooling. I had a colleague in electrical engineering and I remember him telling me at lunch one day that there were many problems in the microelectronics industry related to interdiffusion between the very thin metal layers and that most of this was controlled by grain boundary diffusion. I looked at him and I said “why not get rid of the grain boundaries?” And he said “how? The single crystal thin film growth was very difficult.” I said “no, make the layer amorphous.”

We tried this strategy and it worked very well. We have some patents on it. The method is used today. The transition from aluminum metallization to copper metallization requires a very strong diffusion barrier to the silicon because copper impurities in silicon destroy the semiconducting performance. It was very exciting to be able to do that. This experience shows another very important aspect of materials science in that you study in one area, but the principles and the experience can be applied in many other areas. For example, I serve on Ph.D. committees in pharmacy.

K: In pharmacy?

P: It turns out that the companies that make drugs often use amorphous materials because in the amorphous state they can get more homogenous mixing of the components in the drug. They worry about the effect of moisture on changing the glass transition and causing crystallization. In other aspects, some of the structures that make up these drugs have different possible crystal structures; they are called polymorphs. Each polymorph will react differently with our bodies.

K: It depends on what kind of function is there.

P: Yes, a function is related directly to the structure and the composition. It is important to be able to identify clear ways of making different structures.

K: Very interesting.

P: I have also served on a Ph.D. committee for a student who was studying candy. Many candies are wrapped in cellophane and when you pull the wrapper, the cellophane should come off easily. But if the cellophane is moist, it sticks. This is because the candy picks up moisture from the air and changes the glass transition temperature. I learned much about amorphous materials by serving on these different committees. This shows you how broad an application is working with glasses, because we do not appreciate that many of the materials we work with are actually amorphous. The drugs that we take for health and the sweets that we enjoy for treats are all often amorphous.

K: Yeah, chocolate might be…

P: Chocolate, this is another interesting example. Chocolate that we buy in the store is in a metastable phase. On a hot summer day you can often get little white spots to form on the chocolate. This occurs because the metastable phase is transforming to a stable phase which has a white color. The chocolate companies do not like this because the chocolate has to last on the shelf many months without change.

K: I see. They have to prevent this whitening.

P: When chocolate is made, it is cooled fast enough to get the preferred metastable phase. Chocolate is a very complex, multi-component material and the taste is related to how fine grained this metastable phase is produced.

K: Maybe amorphous.

P: Well, not the chocolate, the metastable phase has different grain sizes. The tongue is very sensitive for not just taste but also for feeling.

K: Yes, indeed. Very interesting.

P: It has been very exciting to learn about new fields and see how the principles from my field can be applied.

K: So your title of Ph.D. thesis was…

P: It was ‘Massive Transformations in Silver-Aluminum System.’

K: This brings you to understand similar phenomena on the basis of your experiments and the interpretation.

P: Exactly. This illustrates some of the principles of research. The trend that is happening today of more and more expansion of interdisciplinary activities, I think, is an important one but we should be careful because you become diluted. There are still some very core subjects that must be covered. For example, there is a very popular trend to go to biological materials.

With metals, ceramics, and polymers, we can deal with common types of structure types and processing. When you consider the biological molecules, there is a whole new language which you must learn; the biological terms. This is similar to learning a new language but then once you learn this you see, all the principles are really similar; transport between cells, nucleation of cells.

K: OK, maybe one thing is a bit different from metallurgy is that they are using water. Without water, no biological materials. That is quite a big difference.

P: It is a quite big difference, right. The interface between biological materials and inorganic materials is the key to controlling function. The compatibility is controlled by the interactions between the water molecules and inorganic materials.

K: This is a kind of a new field which technologists have never experienced for a long time.

P: Right, but at the same time biologists have never considered our field. It is like two strangers are meeting.

K: Yeah, this combination should be very productive in the future.

P: We hope so, yes. We certainly hope so. But I think we have to keep in mind that the basic core principles in the field must be retained. This is very important. The body works because of certain chemistry and certain material reactions that allow you take in food and make energy.

K: And also membrane is a sort of a critical value.

P: Right.

K: We have to go through.

P: I know one of the important applications of bulk metallic glasses that Professor Inoue is looking at relates to using it medical applications, like dental applications where the BMG offers high performance, good compatibility with the body, and low corrosion. They are very important.

K: And you have found several things but please tell us your exciting findings here.

P: I think this use of amorphous metals, as diffusion barriers in microelectronics is one example.

K: You have got it patented already.

P: Yes, I have a patent on it but this was a brand new application in amorphous materials.

K: How did you find this? There must be several difficulties you have to cross over.

P: Yes, the first was in trying to understand the details. Most of the work on materials in this field has been done by electrical engineers who may have a poor understanding of material science. They start with silicon and then they have aluminum on it or copper. During operation they see reactions between the layers. Their approach is put something between the reacting layers.

K: OK and they do not know about the phase diagram.

P: Right. They do not understand the phase diagram. They put another metal between the layers and they get other reactions. Their solution is to add so that instead

of having two metals, they put three, four. They keep adding complexity. When I looked at the problem, I decided that you do not want to add complexity, but you want to simplify the system because in terms of industrial applications or in terms of reliability, fewer components is better.

K: Yes, sure.

P: I also recognized the grain boundary transport is very important in thin films. I said we have to remove that and simplify.

K: By the way, copper is very easy to diffuse in the silicon maybe.

P: That is correct.

K: So it was used for decoration or dislocation sometimes.

P: Exactly. In order to get the extra performance copper is used because it has a lower electrical resistivity than aluminum so there is less heat generated. Modern microelectronics have a high component density. Even though the current is very small in each component over a time the heat builds up. For example, my laptop is too warm for my lap.

K: And heat dissipation is very important, efficient heat dissipation.

P: Exactly. You can improve the performance of materials by reducing the inefficiency.

K: Yes, heat is generated in vain.

P: Exactly. That is waste. With all the concern about energy, efficiency is important.

K: That is right.

P: For example, people are talking about the new sources of energy, but the easiest source of energy is to make less waste then we have more useful energy. I think the metallic glasses can contribute to that in a very important way because they have many functions in magnetic and electrical properties which can be very attractive. They are truly multi-functional, not just structural but other functions.

K: Not excavated yet.

P: Not completely. I think the future is still very bright.

K: Nice expectation.

P: Thank you.

K: So what is your principles or motto which when you come across a difficulty?

P: Well, one of the important lessons I try to give to students when they come to me with their results is to have them ask the right questions.

K: Yes, right question is important.

P: You have an understanding of the past experience from the literature. From this knowledge you should be able to formulate a critical question or hypothesis. If this is true then maybe that is true. I will test this. That is my hypothesis and I will test it. You have to have some working hypothesis. Often students will say, “Well, I am not sure, it could be this or it could be that.” I will tell them, “That is your question?”

K: Just try and find out.

P: Exactly. Because if you ask a good question, the result will always be maybe not the answer you are expecting but a new result.

K: Yes, indeed. Good questions lead to good results.

P: Exactly. That is the most important lesson for students because they read in textbooks the facts and the analysis of those facts is very clear. If you do not have the end of the chapter, just the beginning, how do you get to the end? That is the lesson to teach students and that is why graduate education is more than just lectures and classroom or reading books. It is working with your faculty advisor to learn how to formulate these questions and how to design experiments to answer those questions.

K: How to sort out your experiments and what you extract from…

P: Exactly.

K: By your own eyes.

P: A message to the next generation is, that I think there is a bright future in materials and many new properties to be discovered. Ten years ago we did not have these special materials we have today. I think I should point it out in the biological area there will be many new advances. We will see benefits of joining of material science and biology.

K: However, in general the number of students interested in science has been diminishing. So what can you say or what can you do to the people to get interested in science and technology.

P: I think each one of us must make a commitment to reach out. I know in my laboratory I have actually high school students who work with my graduate students.

K: Oh, really?

P: Yes. We have a program for the summer where the high school student is given registration as a special student. Then, they work in my laboratory next to my graduate students.

K: How many days?

P: They work for the summer period. I have had four students work for us. One came back to material science as a major. My wife is a school teacher. She teaches second grade and the one thing I noticed is that the young children are all scientists. They have a natural curiosity, they want to seek answers.

K: That is very important.

P: They are always touching and examining.

K: That is right.

P: But then when they get older it is beaten out of them somehow.

K: Something wrong in education maybe.

P: Our education system maybe is too rigid. "You must learn just this but what about that? No, no."

K: Non-elastic.

P: We have a fixed direction but curiosity and to ask questions what is this, what is that – no, we ask only certain questions.

K: That is right.

P: You have to learn this. I will give you exam on only this.

K: Your wife studied science?

P: Education. One of my daughters, my older daughter is a biomedical engineer. She works with materials. I have two younger daughters who are going to college now.

K: I also got three daughters.

P: It is wonderful.

K: Yes, three daughters are wonderful.

P: When I give demonstrations to my wife's class and it is very exciting to see the students' reaction to them.

K: Yes. They have a pure interest about science or technology or nature.

P: We have programs in our university where the public schools come to our campus and visit laboratories. We have a public open house where our students make exhibits that the public can come and see.

K: How many high schools boys or girls?

P: In Madison or in…?

K: To this summer school.

P: Oh, the summer school.

K: About 50 or 30?

P: Yes. About 50 and we also have a program for teachers.

K: Oh, even teachers, school teachers?

P: Yes, to come to the university and upgrade their understanding.

K: And you show the laboratories and equipments.

P: Exactly.

K: Dr. Max Lagally is also…

P: Yes, Professor Lagally is in my department.

K: A colleague?

P: Yes.

K: I see. He will also join the summer school.

P: Well, it is run mainly by the students but I know Professor Lagally gives demonstrations and I have given demonstrations as well.

K: Every professor?

P: It is an individual choice. There are formal programs that are again very rigid in their objective. I want more flexibility. I think that is important.

K: And you can sometimes learn from the amateur new things. Their question is really important.

P: Absolutely. I think you are absolutely correct. In the United States the number of students entering science and engineering has been decreasing and there are all these concerns about trying to improve that.

K: Yes, and of course scientists or engineering technology should be paid much better than the modern literature because salary is important.

P: Well, the benefit to society – in our world today we live in a technological society, the benefits are enormous.

K: So they have to pay a lot to the scientists or engineers, if they are very good.

P: We would hope so. I think this WPI program in Japan is an excellent example of the directions to the future because again we have many cultures coming together in this common science. You get different perspectives and influence on this theme that enhances the performance of each person and the output. During my recent visit to Sendai I enjoyed working with the staff. I have a postdoctoral fellow who I worked with closely but I enjoyed working with other students, graduate students and post-docs in the institute and it was very nice. It is a very open atmosphere and you work very hard.

K: Scientific world must be enjoyable, not be forced, but enjoyable, from bottom of the heart, open heart, open discussion.

P: Right.

K: And our life is nothing if it is too laborious and nothing gained. Then, nobody wants to come to the science.

P: It is very satisfying to be able to ask the right questions and see the answers come and then have this deeper understanding and say, oh now we can do this and it works. Wow, that is great. That really is great.

K: Right. You do have a hobby or you like sports or reading or history.

P: I enjoy gardening.

K: Oh gardening, good. You have a big garden in Wisconsin?

P: A reasonable garden.

K: Flowers?

P: Mainly vegetables. We also have some special flowers and some fruit trees.

K: OK, all of your family works together?

P: Yes, my children work with me and they keep the garden watered when I am away but we all enjoy the fresh vegetables in the summertime.

K: Very good.

P: And I enjoy going to symphonies. I wish I had more time to do more but…

K: Do you play yourself?

P: No.

K: OK, and what sort of symphony do you like?

P: Classical.

K: Yes, such as, composer?

P: Bach, and Mozart, and Beethoven.

K: Beethoven is your favorite or Mozart?

P: There is no special favorite. They are all good. Now reading, it is nice to be able to read outside of science.

K: Yes, sure. You have to sometimes relax your brain.

P: It also gives you a better understanding of how people view some things. Often I think science has become too political in this world. The politicians think that they know how to make science work but I am sorry to say that they do not..

K: I am sorry too.

P: I do not feel that they have the proper training and credentials to make scientific decisions, but unfortunately the money that they decide to direct to certain areas determines the science.

K: Money is very, very deficit.

P: I think one of the important lessons for the future is that we must have a long view of science. If it takes 10 years to achieve an objective then it cannot be achieved in 2 years with five times the amount of money. You cannot shorten time with extra money. It still takes time for people to understand. The politicians do not understand this.

K: They say just the amount of money can make everything clear. No, it is impossible.

P: There are big programs in energy now with large amounts of money and they want to see fast results.

K: So to do this carefully we have to know the nature of product globally. Humankind is too selfish for the total biological world.

P: Well, I think this global view is one of the benefits of the WPI. It brings together many different groups like here in Grenoble, France, we have a little bit of Sendai.

K: Sure. What sort of book are you interested in?

P: Mostly true stories.

K: True stories, documentaries.

P: Yes, documentaries of events. I recently read some books on how business works in the stock market and Wall Street because I was curious about these people who get such large bonuses and how they do their job. I had no idea how they make these deals and it is very strange to me that they should make so much money.

K: It started from your curiosity just like science.

P: Exactly.

K: “What mechanism basically working?”

P: So I think we have covered everything.

K: We have covered almost everything. Thank you very much.

P: Yes, thank you.

K: I really enjoyed talking with you.

P: It is really enjoyable and I look forward to continuing my work with the WPI.

Interviewer: Prof. H. Komtasu
in the lobby of Hôtel Angleterre in Grenoble, August 25th, 2009

News Update

Dr. Yamamoto's 2008 Chemical Review paper is selected as a featured New Hot Paper

We are happy to forward you a note by Thomson Reuters (ISI) to Yoshi Yamamoto, our WPI Director, informing that one of his 2008 paper (Nitin T. Patil and Yoshinori Yamamoto, “Coinage metal-assisted synthesis of heterocycles,” Chem. Rev. 108, pp. 3395–3442 (2008)) was selected as a featured New Hot Paper, being one of the most-cited papers (as you see below).

“Science Watch” is a bi-monthly periodical published by Thomson Reuters with wide circulations in global science community.

The citation profiles of Drs. Y. Yamamoto and M. Kawasaki, two highly cited researchers of WPI-AIMR, follows just for your information.

Sent: Wednesday, November 25, 2009 5:08 AM
To: yoshi@mail.tains.tohoku.ac.jp
Subject: Thomson Reuters ScienceWatch has selected your article as a featured **New Hot Paper.**

Dear Dr. Yoshinori Yamamoto,

We are pleased to inform you that your article entitled “Coinage metal-assisted synthesis of heterocycles,” as published in the journal *CHEMICAL REVIEWS* in August, 2008, has been identified by **Thomson Reuters *Essential Science Indicators*** as a featured **New Hot Paper** in the field of Chemistry, which means it is one of the most-cited papers in its discipline published during the past two years.

We are asking for your comments as corresponding author on the following questions and we would like to add your response to the **Thomson Reuters Science Watch** website on Monday, January 4, 2009 at the following link: http://www.sciencewatch.com/. You may reply directly using this email.

Please be sure to include your current title and affiliation along with a personal photo (in .jpg, .gif, .bmp, .png, or tiff formats) which will be used to accompany your commentary. You may also choose to provide as many as three images [along with text descriptions] which describe your research.

Essential Science Indicators is a resource that enables researchers to conduct ongoing, quantitative analyses of research performance and track trends in science. Covering a multidisciplinary selection of 11,000+journals from around the world, this in-depth analytical tool offers data for ranking scientists, institutions, countries, and journals.

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Yours Sincerely,
Doug Benson
Data Coordinator, *Essential Science Indicators*
Thomson Reuters

Citation of Y. Yamamoto

November 2009

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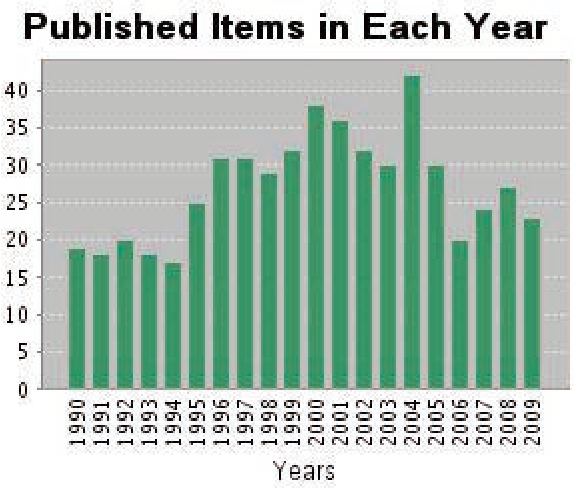

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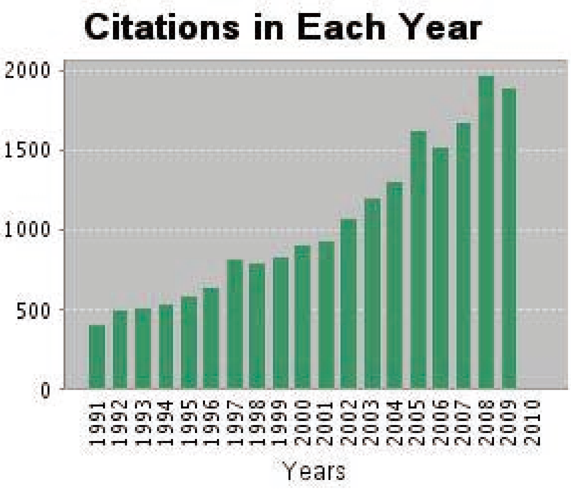

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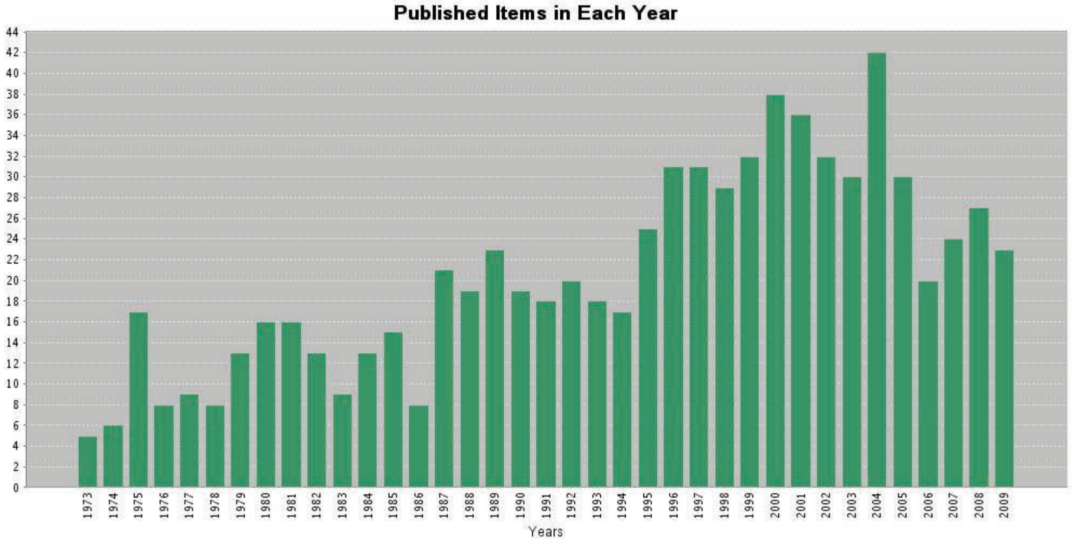

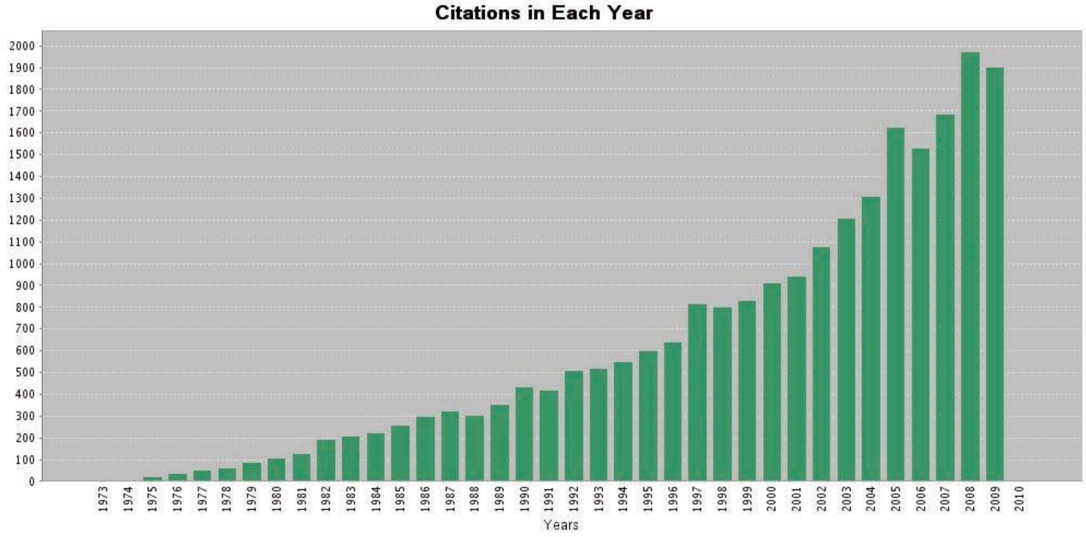

Citation of Y. Yamamoto
November 2009

	AU	TI	Source, Volume, page and year	Document Type	TC
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2	Saito, S; Yamamoto, Y	Recent advances in the transition-metal-catalyzed regioselective approaches to polysubstituted benzene derivatives	Chem. Rev. 100, 2901 (2000).	Review	429
3	Nakamura, I; Yamamoto, Y	Transition-metal-catalyzed reactions in heterocyclic synthesis	Chem. Rev. 104, 2127 (2004).	Review	409
4	YAMAMOTO, Y	ACYCLIC STEREOCONTROL VIA ALLYLIC ORGANOMETALLIC COMPOUNDS	Accounts Chem. Res. 20, 243 (1987).	Review	331
5	YAMAMOTO, Y	SELECTIVE SYNTHESIS BY USE OF LEWIS-ACIDS IN THE PRESENCE OF ORGANOCOPPER AND RELATED REAGENTS	Angew. Chem.-Int. Edit. Engl. 25, 947 (1986).	Article	258
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11	Asao, N; Takahashi, K; Lee, S; Kasahara, T; Yamamoto, Y	AuCl3-catalyzed benzannulation: Synthesis of naphthyl ketone derivatives from o-alkynylbenzaldehydes with alkynes	J. Am. Chem. Soc. 124, 12650 (2002).	Article	167
12	Nakamura, H; Iwama, H; Yamamoto, Y	Palladium- and platinum-catalyzed addition of aldehydes and imines with allylstannanes. Chemoselective allylation of imines in the presence of aldehydes	J. Am. Chem. Soc. 118, 6641 (1996).	Article	165
13	Nakamura, I; Yamamoto, Y	Transition metal-catalyzed reactions of methylenecyclopropanes	Adv. Synth. Catal. 344, 111 (2002).	Review	150
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24	YAMAMOTO, Y; YAMAMOTO, S; YATAGAI, H; MARUYAMA, K	LEWIS ACID MEDIATED REACTIONS OF ORGANOCOPPER REAGENTS - A REMARKABLY ENHANCED REGIOSELECTIVE GAMMA-ATTACK OF ALLYLIC HALIDES AND DIRECT ALKYLATION OF ALLYLIC ALCOHOLS VIA RCU-BF3 SYSTEM	J. Am. Chem. Soc. 102, 2318 (1980).	Article	108
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26	Yoshikawa, E; Radhakrishnan, KV; Yamamoto, Y	Palladium-catalyzed controlled carbopalladation of benzyne	J. Am. Chem. Soc. 122, 7280 (2000).	Article	102
27	YATAGAI, H; YAMAMOTO, Y; MARUYAMA, K	A NEW PROCEDURE FOR THE STEREOSELECTIVE SYNTHESIS OF (Z)-2-ALKENYLSILANES AND ALKENYL-TINS AND THEIR APPLICATION TO ERYTHRO-SELECTIVE SYNTHESIS OF BETA-ALKYL ALCOHOL DERIVATIVES	J. Am. Chem. Soc. 102, 4548 (1980).	Note	102
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29	TAMARU, Y; YAMADA, Y; INOUE, K; YAMAMOTO, Y; YOSHIDA, Z	OXIDATION OF PRIMARY AND SECONDARY ALCOHOLS BY THE CATALYSIS OF PALLADIUM	J. Org. Chem. 48, 1286 (1983).	Article	101
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32	Nakamura, I; Itagaki, H; Yamamoto, Y	Ring opening in the hydroamination of methylenecyclopropanes catalyzed by palladium	J. Org. Chem. 63, 6458 (1998).	Letter	92
33	YAMAMOTO, Y; MARUYAMA, K	ZIRCONIUM ENOLATES AS A NEW ERYTHRO-SELECTIVE ALDOL CONDENSATION REAGENT	Tetrahedron Lett. 21, 4607 (1980).	Article	91
34	Nakamura, K; Nakamura, H; Yamamoto, Y	Chiral pi-allylpalladium-catalyzed asymmetric allylation of imines: Replacement of allylstannanes by allylsilanes	J. Org. Chem. 64, 2614 (1999).	Letter	88
35	Camacho, DH; Nakamura, I; Saito, S; Yamamoto, Y	Palladium-catalyzed addition of alcohol pronucleophiles to alkylidenecyclopropanes	J. Org. Chem. 66, 270 (2001).	Article	83
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39	Ibuka, T; Mimura, N; Aoyama, H; Akaji, M; Ohno, H; Miwa, Y; Taga, T; Nakai, K; Tamamura, H; Fujii, N; Yamamoto, Y	A thermodynamic preference of chiral N-methanesulfonyl and N-arenesulfonyl 2,3-cis-3-alkyl-2-vinylaziridines over their 2,3-trans-isomers: Useful palladium(0)-catalyzed equilibration reactions for the synthesis of (E)-alkene dipeptide isosteres	J. Org. Chem. 62, 999 (1997).	Review	81
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42	OGAWA, H; ONITSUKA, K; JOH, T; TAKAHASHI, S; YAMAMOTO, Y; YAMAZAKI, H	SYNTHESIS, CHARACTERIZATION, AND MOLECULAR-STRUCTURE OF MU-ETHYNEDIYL COMPLEXES [X(PR3)MC=CM(PR3)2X] (M = PD, PT, R = ME, ET, N-BU, X = CL, I)	Organometallics 7, 2257 (1988).	Article	80
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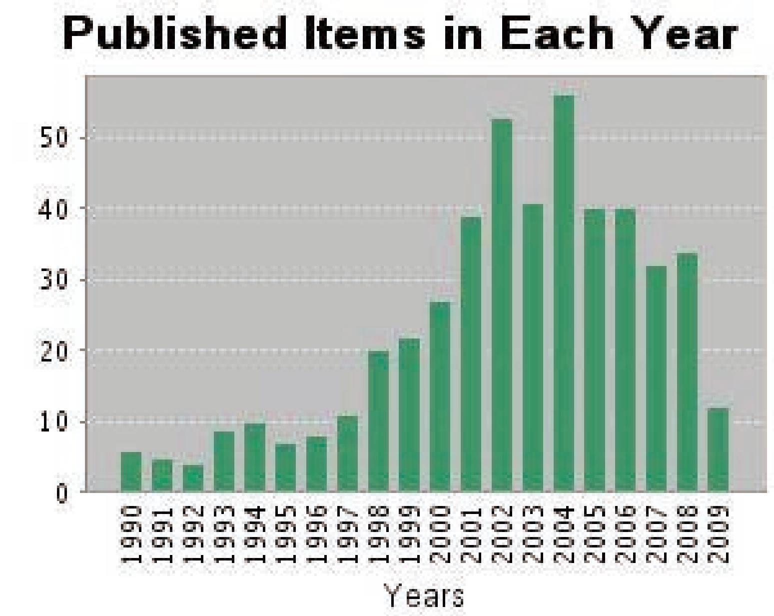

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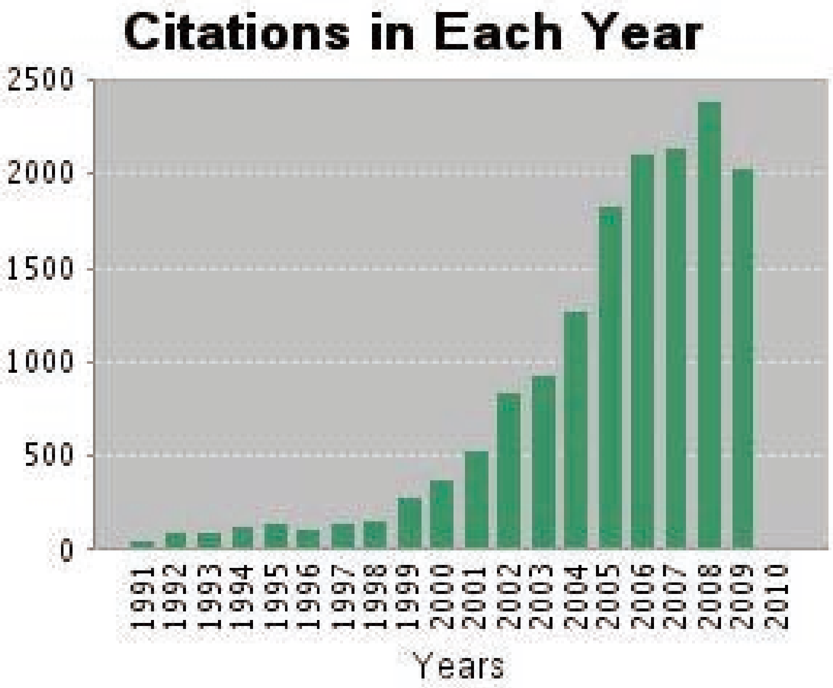

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	AU	TI	Source, volume, page and year	Document type	TC
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Funding Program for World-Leading Innovative R&D on Science and Technology.
“Research and development of integrated microsystems.”

Masayoshi Esashi
WPI-AIMR, Tohoku University, Sendai 980-8579, Japan

Thirty researchers were chosen in Japan for the Funding Program for World-Leading Innovative R&D on Science and Technology. Prof. Hideo Ohno (Spintronics) in the Research Institute for Electrical Communication and Prof. Masayoshi Esashi (Integrated microsystems) are the principle researches from Tohoku University. The term and the budget of this program are 2009~2013 (fiscal year) and ~5M$ / year respectively.

The program of the “integrated microsystems” is the collaboration with Dr. Ryutaro Maeda in Advanced Manufacturing Research Institute (AMRI) in National Institute of Advanced Industrial Science and Technology (AIST) in Tsukuba. Supporting the competitiveness of industry is aimed based on the technology called MEMS (Micro Electro Mechanical Systems). Social problems as aging and preserving environment and industrial problems as the economical crisis of advanced LSI are expected to be solved in the program by the following approach.

「Heterogeneous integration」 to integrated heterogeneous components for value added devices.

「Hands-on access to fab.」 for lowering the barrier to start development without own facility.

「Shared wafer」 for MEMS processes on LSI to minimize risks in R&D by reducing a development cost.

「Development of massive parallel electron beam exposure systems」to produce small volume advanced LSI cost effectively.

「Fundamental technology for sensor-net green-fab.」 to preserve environment and to save energy.

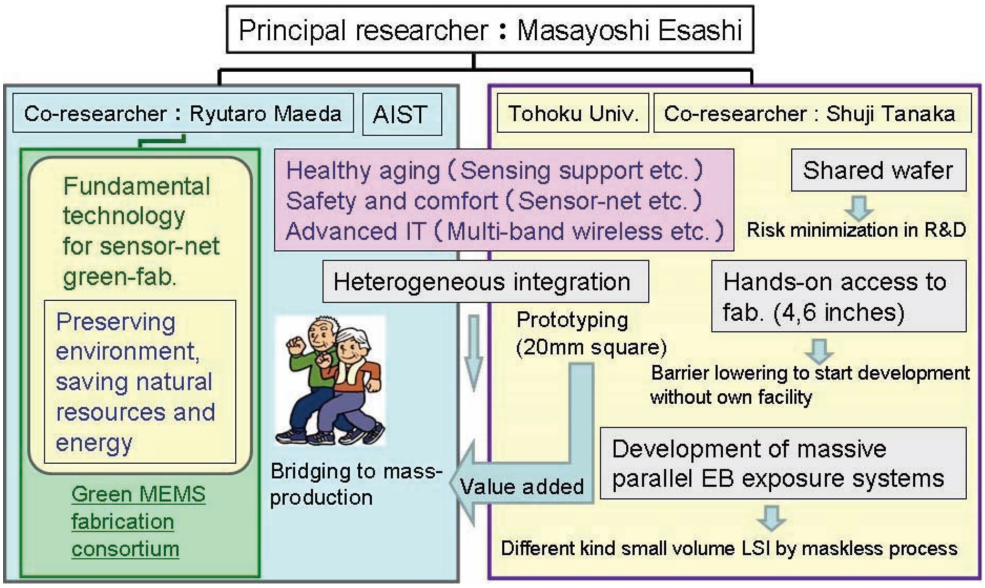

Fig.1 Scheme of the research and development of integrated microsystems

The New WPI Joint Seminar Series

by M. Tsukada and T. Hashizume

The 11th Seminar Oct. 23 (Fri.) 16:00~17:00

Prof. Weihua Wang (Institute of Physics, CAS, Beijing):

"Microalloying induced giant properties & GFA change in BMGs"

The 12th Seminar Oct. 30 (Fri.) 15:00~17:20

Dr. Tsuneya Ando (Tokyo Inst. of Technology):

"Physics of graphene and its multilayers: From zero-mode anomalies to band-gap opening"

Dr. Keith McKenna (WPI-AIMR):

"Electronic and optical properties of polycrystalline metal-oxide materials"

The 13th Seminar Nov. 6 (Fri.) 15:00~17:00

Prof. Andreas Züttel (EMPA Materials Sciences and Technology):

"What We Learn From The Past To Master The Future With H_2"

Prof. Shin-ichi Orimo (IMR, Tohoku University):

"Metal Borohydrides for Energy Applications"

The 14th Seminar Nov. 20 (Fri.) 15:00~17:00

Dr. Katsuya Iwaya (WPI-AIMR):

"Tutorial to Scanning Tunneling Microscopy (STM)"

Dr. Terukazu Nishizaki (IMR, Tohoku University):

"Low-temperature STM studies on superconductors"

Prof. Taro Hitosugi (WPI-AIMR):

"Introduction to low temperature SPM at WPI-AIMR"

The 15th Seminar Dec. 18 (Fri.) 15:00~17:00

Dr. Ali Khademhosseini (Harvard Medical School):

"Microengineered hydrogels for stem cell bioengineering and tissue regeneration"

Dr. Douglas B. Weibel (University of Wisconsin-Madison):

"Transforming Microbiology Using Soft, Biocompatible Polymers"

Research Prospect

MEMS with new functional materials

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1. MEMS bonding technologies

Recent advances in commercialization of micro electro mechanical systems (MEMS) products rely on development of integration technologies for packaging, combining MEMS with integrated circuit or other systems, and to realize 3d device stacking. Bonding technology is the key for wafer level packaging and 3d integration, and is getting more and more significance for MEMS device. For an industrial MEMS device [1-3] more than 70 % costs come from bonding process and its evaluation. Wafer bonding technology got its start in the manufacture of MEMS, for protection and sealing purposes of fragile MEMS structures, also for a interconnection between top and bottom wafers. Especially for novel consumer MEMS applications, such as Apple iPhone or the Nintendo Wii, that have to keep record-small form factors, wafer bonding is a major contributor to reduce the manufacturing costs of the final package. New bonding schemes for wafer-level-packages (protection, interconnection and testing at the wafer level) are being discussed with regards to market potential and equipment requirements.

The successful technology transfer of wafer bonding and related advanced manufacturing technologies from MEMS packaging into 3D wafer stacking of CMOS based applications [1]. Recent development of wafer level bonding to combine MEMS device with LSI decreases size and cost significantly and exhibits low electrical noise. Bonding technology with temperature below 400 ℃ and achieve both mechanical and electrical bonding at the same time have been paid large attention and is a critical issue for practice application. Table 1 shows the overview of MEMS wafer bonding technology. Only a few bonding choices can satisfy sealing packaging and electrical bonding at the same time. In which, some technical problems are always need to challenge, such as strength of the bonds, bond yield, adhesion with both sides wafers etc.

In this study, bonding technology with metallic glass [4-5] has been proposed to create a new bonding technique field. In addition of using new bonding materials, nanostructured [6-7] metal pads have also considered to achieve low temperature bonding and provide a conductive functionality to anodic bonding, the most used bonding method for device encapsulation.

Table 1. Overview of MEMS wafer bonding technology (WBT).

		WBT with intermediate layer				WBT without intermediate layer	
		Eutectic bonding	Diffusion bonding	Glass frit bonding	Polymer	Anodic bonding	Si direct bonding
		Electric conductive		Non electric conductive			Plasma bonding
Bonding temperature		190-380	300-400	400-550	250-350 / 120-160	350-400	RT-300
Electrical connection		○	○	×	×	×	×
Mechanical hermetic sealing	Low vacuum	○	○	○	○ / ×	○	○
	High vacuum	○	○	×	×	○	○
Alignment accuracy (μm)		< 2	< 2	< 10	< 2 / < 5	< 2	< 2
Surface roughness requirement		μm	nm	μm	μm	< 10nm	< 1nm

1.1 MEMS bonding with AuSi

Eutectic bonding has got a special importance today because both hermetically sealed package and electrical interconnects could be performed within one process. Furthermore, there are some advantages such as low processing temperature, low resultant stress induced in the final assembly, high strength of the bonding, large fabrication yield, and a good reliability.

Since the early 90-ies eutectic bonding is known from very large scale integration (VLSI) chip bonding and is used very often in industry. The AuSi eutectic bond process is a well known technique in the field of single chip packaging. The bond mechanism relies on the formation of eutectics at the interface. The AuSi eutectic bonding dramatically decreases the process temperature to be under 400°C, provides good mechanical stability, and has availability in micro technologies.

Wafer-to-wafer AuSi eutectic bonding has been investigated in our group [8-9]. Single crystalline Si, amorphous Si and poly crystalline Si were bonded with Au layers and observed by optical measurements. Material composition, adhesion layer, electrical insulation, bonding parameters, and surface pre-treatments were discussed and have improved bonding performance. Bond strength determined by micro-chevron-test and shear test was evaluated as well as hermeticity. High bond yield was achieved with 4 inch and 6 inch wafer stacks. Figure 1 shows SEM images of 100 % AuSi eutectic bonded 6 inch wafer pairs.

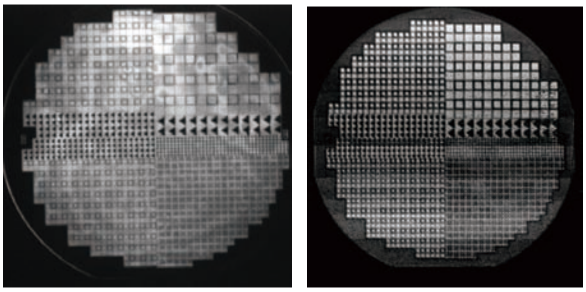

(a) (b)

Figure 1. (a) Infrared images and (b) ultra sonic images of 6 inch AuSi eutectic bonded wafers.

1.2 MEMS bonding with new materials - metallic glasses

The main goal is to develop new MEMS bonding field with metallic glasses. It is expected to achieve unprecedented high-capabilities bonding performance. With creation of a novel bonding technique with metallic glass, the developments of metallic glass deposition technologies are also expected to become as MEMS compatible fabrication processes to open further MEMS application with metallic glass materials simultaneously. This research will not only show the possibility but also challenge the conventional MEMS bonding field.

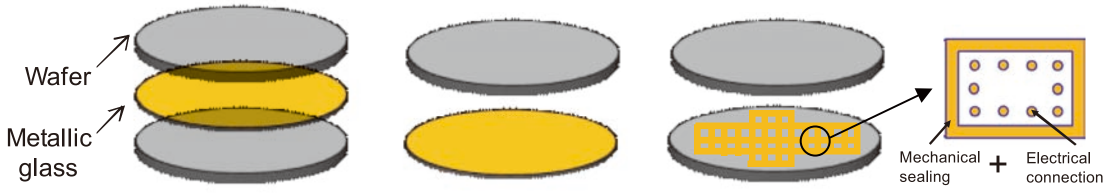
Metallic glass with superior material properties, e.g. tough, anticorrosion, glass transition behavior and material variegation, has be considered as a candidate of novel bonding material. As a MEMS bonding material, metallic glass is like a mixture of eutectic bonding and glass frit bonding. During bonding process, the apply temperature above its glass transition temperature (T_g) exhibits a low temperature bonding by selection a proper kind of metallic glass.

The requisite properties of bonding materials are adhesion capability with both sides materials, large bond strength, high electrical conductivity, anticorrosion, and MEMS compatible manufacture. Metallic glass is well known with large strength and anticorrosion. It has material variegation and there are already more than 2000 kinds of metallic glass have been developed. By selecting proper base materials, it has high potential to achieve adhesion capability and high electrical conductivity to answer bonding requirements.

At the early stage, the existing metallic glass will be considered and suitable materials will be implemented to show basic experimental tests. Base on these results, novel bonding adaptable metallic glass will be developed in the company of bonding experiments. Bonding parameters such as heating temperature, heating time and pressure are important issues and will be investigated. Standard evaluations will be implemented to show its bonding reliability.

Figure 2 shows the schematic of wafer bonding with metallic glass. The metallic glass can be fabricated into three ways: sheet, full area deposition and patterned fabrication, to achieve full area bonding, on-chip full wafer bonding and local area bonding, respectively. Both mechanical sealing and electrical connection are expected to achieve at the same time.

There are some requirements for metallic glasses candidates such as good adhesion with Si/SiO_2, proper T_g and T_x, easy compositional control of film by sputtering and large supercooled liquid region. The X-ray diffraction curve and DSC (Differential Scanning Calorimeter) curve of sputtered Zr-Al-Cu-Ni thin film are shown in Figure 3. The sputtered Zr-Al-Cu-Ni metallic glass thin film exhibits good adhesion with Si substrate.



(a) (b) (c)

Figure 2. Wafer bonding methods with (a) metallic glass sheet, (b) full wafer deposited metallic glass and (c) patterned metallic glass thin film.

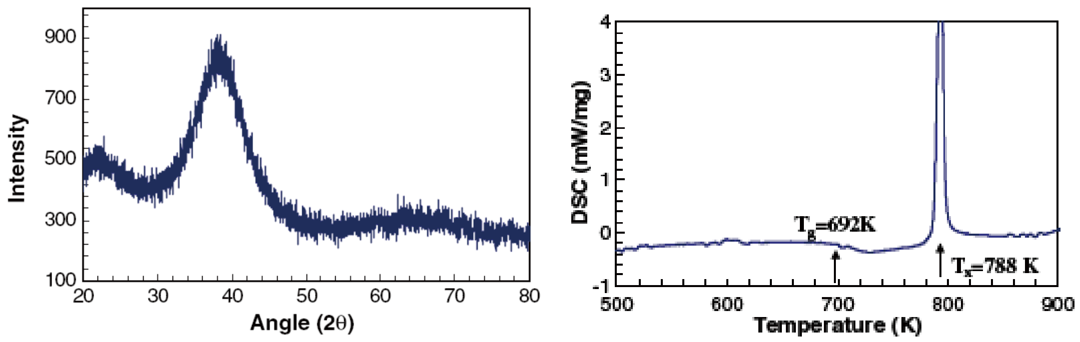


Figure 3. (a) X-ray diffraction curve and (b) DSC curve showing the amorphous nature of sputtered Zr–Al–Cu–Ni thin films [10].

1.3. Nanostructured intermediate layer for MEMS bonding - nanoporous metals

Metallic nano-lawn and Au particles have been identified earlier [11-12] as promising candidates for applications in low temperature bonding. Even if their introduction into technological flow schemes is only about to start, potential applications attractive for advanced packaging have been already demonstrated. For further low cost, simple process, and large area fabrication, nanoporous metals has been proposed in this study.

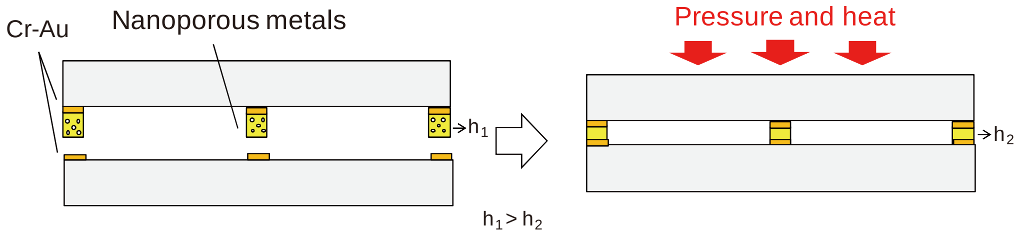
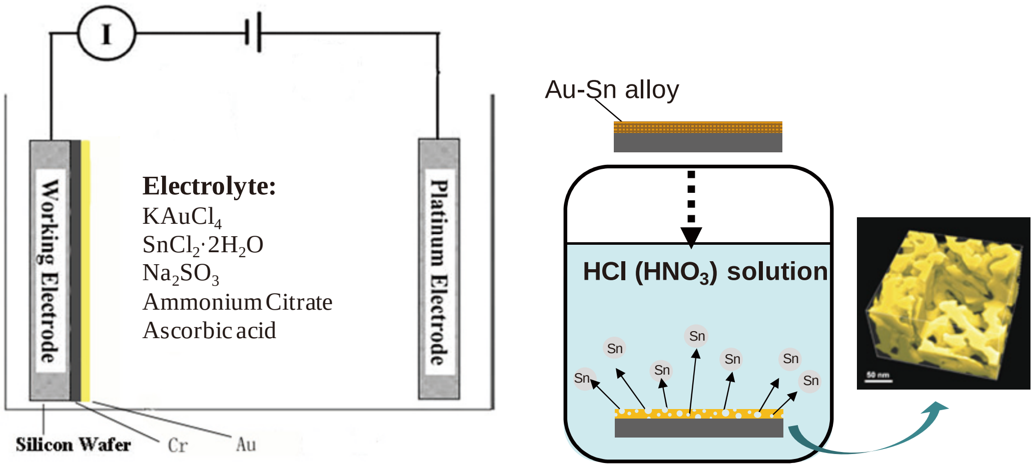


Figure 4. Schematic of wafer bonding with nanoporous structured intermediate layers.

Nano-porous metallic formation has been well developed with sheet style. This technology will be transferred as an on-wafer process and combined with MEMS electrodeposition. Figure 4 shows the schematic of wafer bonding with nanoporous metals. Experimental setting of Au-Sn alloy electrodeposition and dealloying precess are shown in Figure 5.



(a) (b)

Figure 5. Fabrication of nanoporous metals (a) Au-Sn alloy electrodeposition and then (b) dealloying.

1.4 Anodic bonding with conductive functionality

Anodic bonding is popular method for the cap bonding process. Most MEMS cavity packages are hermetically sealed by anodic bonding. However, anodic bonding can not perform electrical conductive functionality that is required for many practical applications. Here, nanostructured metal pads will be fabricated for standard anodic bonding with nanoporous metals and nanostructured metallic glasses to create its electrical conductive functionality for packaging application.

Figure 6 shows schematic of anodic bonding with structured metal pads. The structured metal pads have a larger thickness (h_2) than bonding frame (h_1) to make electric connect surely. When press two wafers together with heat applying, structured metal pads crush and then diffuse into interconnection on both sides without overflow.

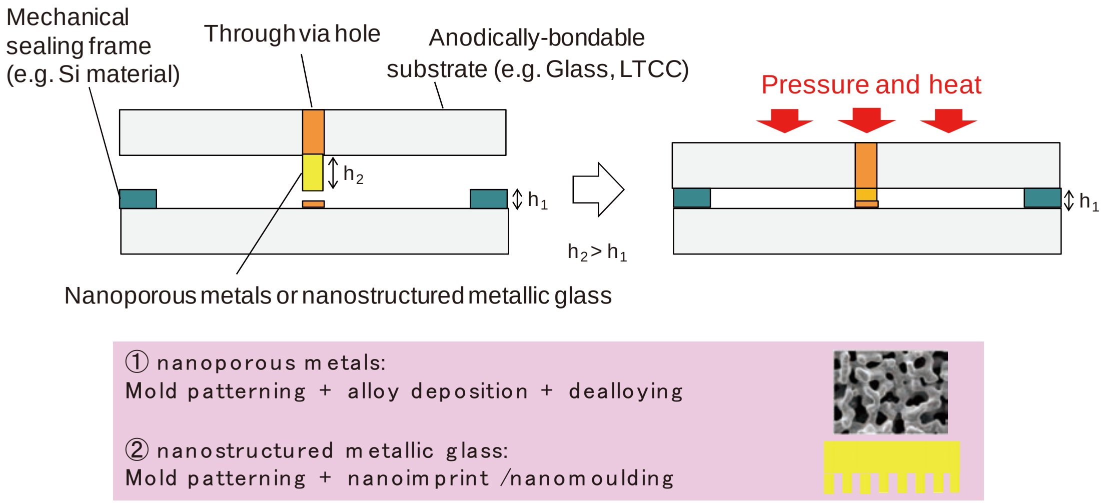
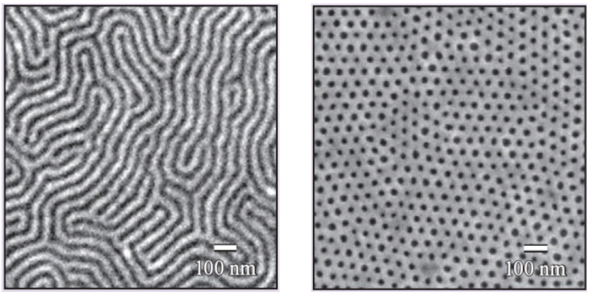


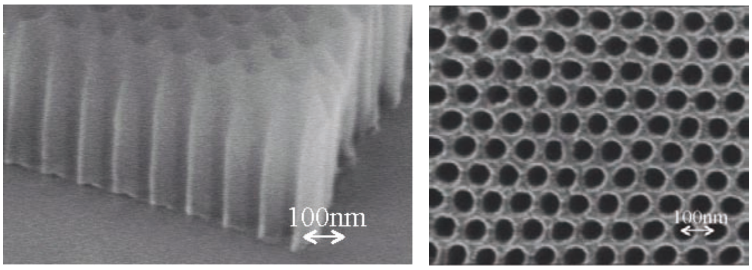
Figure 6. Schematic of anodic bonding with a structured metal pad.

The metal pads can be made with nanoporous metals or nanosturctured metallic glass. Fabrication of nanoporous metals has been described in section 1.3. Nanosturctured metallic glass could be formed by nanoimprint or nanomoulding with supercooled liquid region of metallic glass. The mold nanopatterning is proposed to use self assembling diblock copolymer or porous alumina as substitute resist layers without conventional expensive photo lithography. Figure 7 and 8 show the nanopatterns of diblock copolymer and porous alumina.



(a) (b)

Figure 7. Self assembled nanostructure of diblock copolymer [13]. (a) Surface-parallel-oriented phase PS-b-PMMA diblock copolymer patterns. (b) Surface-perpendicular-oriented cylindrical phase PS-b-PMMA diblock copolymer patterns.



(a) (b)

Figure 8. Pattern transfer from porous alumina to diamond and resist [14]. (a) Porous alumina (b) Diamond mold

2. Fabrication of micro mirrors with metallic glasses

MEMS have been synthesized in a variety of applications from electronics to bio-technology, using advanced micromachining and nanomachining technologies based on the extended semiconductor microfabrication. As an important part of MEMS, micro/nano machine has a critical requirement for materials.

Silicon MEMS devices such as micro-mirrors, however, are prone to early mechanical failure even with a small crack during fabrication, which results from lack of ductility in Si. Also, most prcesses of micro mirror use expensive SOI (Silicon On Insulator) wafers. Continued desires of higher performance, extensive durability and low cost in the sophisticated MEMS devices have been a continuous driving force in search of more advanced MEMS material. Recently, stainless steel was proposed as an alternative to overcome the substrate fragility, nevertheless, the curvature in the substrate induced by residual stresses inhibits its successful replacement of Si. Therefore, a novel material with desirable combination of high strength, good wear-resistance and electrical conductivity with a MEMS-compatible simple process is the key to overcome current bottleneck in MEMS material performance thus to create a new field in MEMS world. Metallic glasses can be shaped at elevated temperatures into various complex forms at a wide variety of scales even down to atomic scale. Moreover, versatility in composition and properties of available MG alloys significantly enhances their promise in MEMS applications.

Mircro scanning mirrors driven by an electrostatic force [15], piezo [16], and magnetic force [17] have been extensively reported. In which electromagnetic actuation is a promising technique to drive microdevices. The noncontact electromagnetic actuator is able to deliver a large force and a large displacement. In this study, metallic glass micro mirror will use a coilless driven actuation [18]. The magnetostatic force resulted from a magnetic interaction as well as the Lorentz force that is induced by an eddy current as shown in Figure 9. The eddy current is exploited here to generate the Lorentz force without conducting wire in an ac magnetic field. Meanwhile, the magnetostatic force will also be induced in the magnetic field to drive the scanner. The eddy current can be induced in metal, particularly ferromagnetic metallic glass materials with higher permeability. This eliminates complicated coil routing and insulation layer deposition and simplifies fabrication allowing easy integration with micromachining and complementary metal–oxide–semiconductor processes.

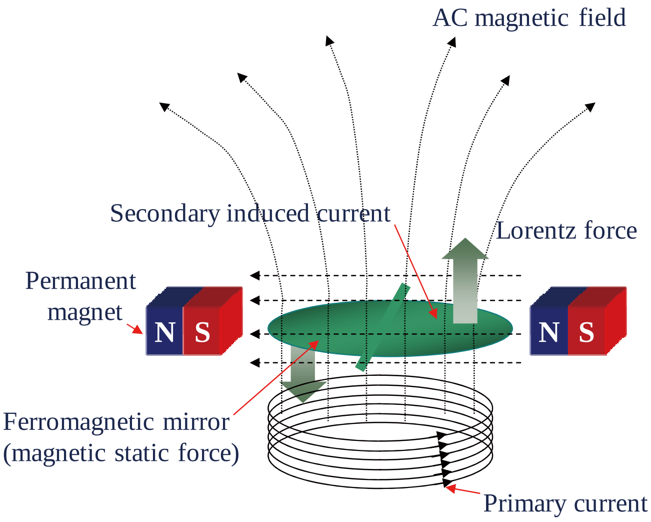
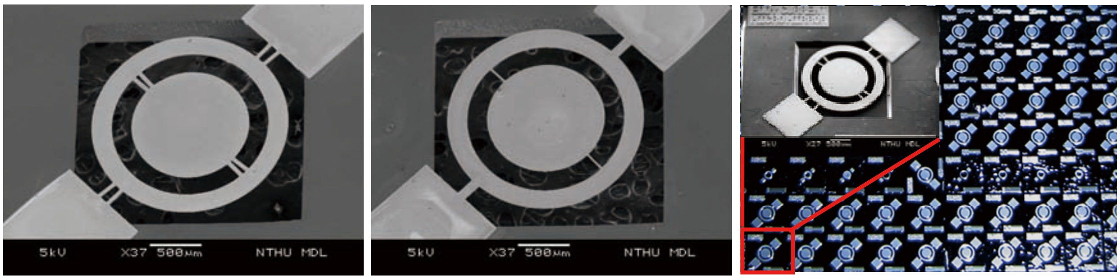


Figure 9. Concept of coil-less MEMS scanning micro mirror.

Two-axis micromachined scanning mirror is a key enabling component for optical applications such as the compact display system. In general, the scanning mirror employs microactuators to manipulate incident light in two orthogonal directions. Thus, the design considerations include large scanning angle, high frequency response, and low driving voltages. Two-dimensional scanning patterns can be easily tuned by varying the combination of driving frequencies. Figure 10 shows typical fabricated micro mirrors.



(a) (b) (c)

Figure 10. SEM images of typical fabricated (a) one-axis, (b) two-axis micro mirrors and mirror array [19].

With fusion of bulk metallic glasses, micro-/nano- device/systems and nanomechanics, this proposed research aims at developing a novel metallic glass micro mirror and MEMS compatible fabrication technologies of metallic glass including moulding and surface planarization, integration with other materials etc. for actuation, control or handling. In addition to search of more advanced material, development of a MEMS-compatible fabrication process is of the most importance to a successful MEMS application with metallic glasses. In light of this desire, this research is expected to make a bridge between metallic glass and MEMS and further innovative applications of metallic glasses and to create a new regime in MEMS.

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Science Based New Silicon Technologies Based on New Manufacturing Equipment Completely Free From Contaminations and Damages

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Abstract

Current silicon technologies are now facing with very severe standstill, i.e., the speed performance of microprocessors can not be improved any more at the current maximum clock rate of 3.8GHz. Current silicon technologies are characterized by the thermal oxidation at high temperatures using O_2 and/or H_2O molecules to form the gate insulator films of MOS transistors, resulting in the fact that relatively high integrity silicon dioxide films (SiO_2) are obtained only on the (100) silicon surface while there are obtained very poor quality oxide films on the other silicon surfaces. Thus, silicon LSI (Large Scale Integration Circuit) can be fabricated only on the (100) silicon surface using two dimensional (2D) structure MOS transistors, so that the very limited capability of the silicon crystal can be used to the practical applications by the current silicon technologies.

The stagnation of the silicon LSI induces very severe standstill of Information and Communication Technologies (ICT), resulting in the standstill of the progress of world-wide entire industries.

In order to overcome these stagnations of silicon technologies, we must develop very new manufacturing technologies to form very high integrity gate insulator films on any crystal orientation silicon surface with the same formation speed based on the radical reactions, resulting in the creation of science based new silicon technologies where very high integrity SiO_2 films and Si_3N_4 films can be formed using oxygen radicals O* and NH* radicals on any crystal orientation silicon surface with the same oxidation speed and the same nitridation speed, so that the three-dimensional (3D) structure MOS transistors are fabricated on any crystal orientation silicon surface. Thus, the entire capability of the silicon crystal will be used to the practical applications where the speed performance of silicon LSI will be improved greater than 100 GHz by introducing balanced CMOS of accumulation mode MOS transistors on the (551) surface SOI wafers, i.e., science based new silicon technologies will start just right now.

1. Introduction

Radical reaction based semiconductor manufacturing has been confirmed to exhibit very high quality process results such as oxidations, nitridations, plasma CVD and reactive ion etching (RIE) by using 2.45 GHz Horn Antenna excited high density plasma with very low electron temperatures (1), where the speed performance of the silicon LSI is speculated to improve greater than 50 GHz clock rate (2). Typical results of radical oxidation and radical nitridation are shown in Fig. 1, where the leakage current densities of current thermal oxide, radical oxide (400℃) and radical nitride (600℃) are plotted as a function of the effective oxide thickness (EOT) for an applied voltage of 1 volt. It has been demonstrated in Fig. 1 that the leakage current density of radical oxide and radical nitride has been improved to decrease down to less than 1/1,000 compared to that of current thermal oxide. But, 2.45 GHz Horn Antenna excited high density plasma can be applied only to the small size substrates such as 5cm to 10cm in diameter. It is very essential for us to develop new plasma process equipment for the very large size substrates in order to introduce these very high quality radical reaction based semiconductor manufacturing to the practical applications because current plasma equipment can not be used to the transistor fabrication in the semiconductor manufacturing due to its very severe contaminations and very severe damages such as the charge-up damages and the ion bombardment induced damages. Thus, current plasma equipment is used

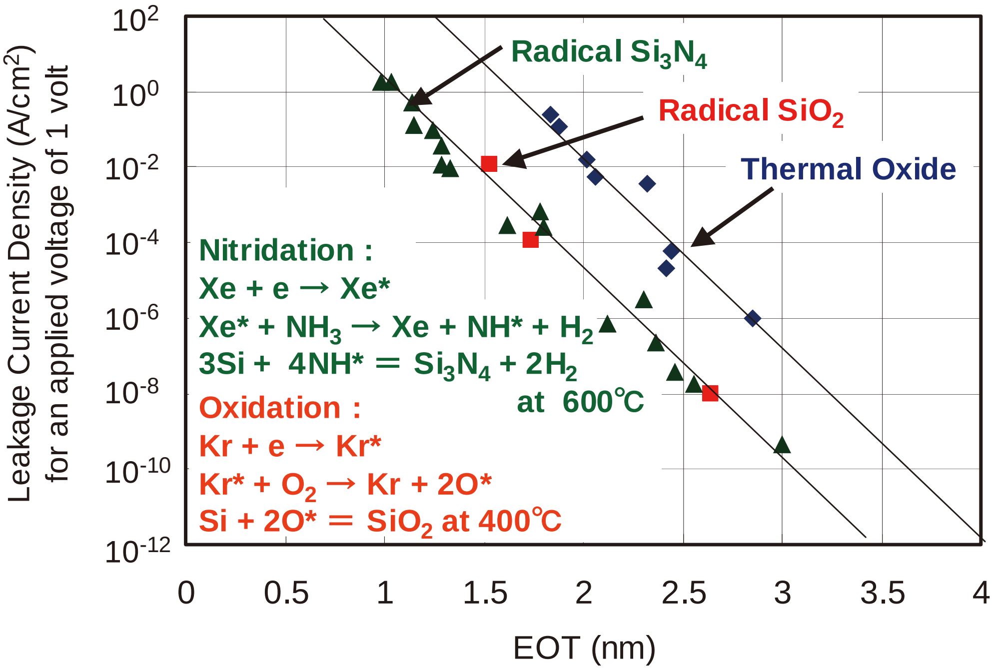


Figure 1 The leakage current densities of current thermal oxide, radical oxide and radical nitride are plotted as a function of effective oxide thickness from 3 nm to 1 nm for an applied voltage of 1 volt.

only to the interconnects fabrications.

We are now developing new plasma process equipment completely free from contaminations and damages such as 915MHz Metal Surfacewave Excitation Plasma (MSEP) with single shower plate structure and dual shower plate structure, and Rotation Magnet Sputtering having very high target utilization efficiency (3). In this paper, we will describe the importance and the practical applications of 915 MHz MSEP. The metal surfacewave is newly discovered propagation mode of the electromagnetic waves propagating along with the plasma sheath region between the metal surface covered with Al_2O_3 passivation film and the high density plasma. In order to obtain the very stable plasma excitation and low electron temperature plasma, the electromagnetic wave must be reflected at the surface of excited plasma, so that the electron density in the plasma excitation region must be completely higher than the cutoff density n_c given by

$$n_c = \frac{m_e \varepsilon_0 \omega^2}{e^2}, \qquad (1)$$

where m_e and e are the electron muss and the electric charge, ε_0 is dielectric constant of the free space and ω is angular frequency. The cutoff electron density of 915MHz is very low such as $1.04\times10^{10}\text{cm}^{-3}$, so that we can obtain very stable plasma excitation even for 100% O_2 gas ambience and 100% F_2 gas ambience at very wide range of working pressures where the oxygen and the fluorine have large electronegativity such as 3.5 and 4.0 resulting in the generation of negative ions by absorbing electrons, i.e., corresponding to the drastic decrease of electron concentrations in the plasma. This clearly indicates that we can obtain very stable and uniform plasma excitation for very wide variety gas combinations and working pressures i.e., very wide process windows.

In order to eliminate charge-up damages and ion bombardment induced damages, the silicon substrates must be set in the diffusion plasma region separated from the plasma excitation region, where the electron current and the ion current flowing into the substrate surface are completely equal to each other at any time, so that the electric charges do not remain at the substrate surface even if the plasma is turned-off at any time. Charge-up damages are principally eliminated by setting the substrate in the diffusion plasma region. To eliminate ion bombardment induced damages, the electron temperature of the diffusion plasma region must be decreased as small as possible, because the bombarding ion energy is given by

$$E_{ion} = \frac{kT_e}{2} \ln\left(\frac{0.43 m_i}{m_e}\right), \qquad (2)$$

where T_e is the electron temperature of the diffusion plasma region, m_i is mass of ion and k is the Boltzmann constant. Typical bombarding ion energy is tabulated in Table 1. The electron temperature must be decreased down to less than 2.0 eV, so that higher frequency plasma excitation is essentially required such as 915 MHz.

By decreasing the electron temperature of the diffusion plasma region, the bombarding ion energy becomes very small, so that we can introduce the lower shower plate supplying various process gases to the diffusion plasma region without suffering sputtering. Various process gases are supplied to the substrate surface through the diffusion plasma region having very low electron temperatures, so that process gas molecules do not decompose even if they suffer electron collisions. Thus, process gas molecules can reach to the bottom of very narrow and very deep throughholes without absorbing to the inlet sidewall of these throughholes, resulting in the same etching speed to the entire pattern sizes as shown in Fig. 2. Current plasma equipment exhibits very severe pattern size dependence of the process speed as shown in Fig. 2, where the etching speed strictly decreases with a progress of pattern size miniaturization.

Table 1 Table 1 Bombarding ion energy to the substrate surface of various electron temperature of the diffusion plasma region for various ions from H^+ to Xe^+.

T_e Ion	2.0eV	1.5eV	1.0eV	0.7eV
H^+ (1)	6.8	5.1	3.4	2.4
He^+ (4)	8.1	6.1	4.1	2.9
N^+ (14)	9.4	7.0	4.7	3.3
SiH_2^+ (30)	10.2	7.6	5.1	3.6
Ar^+ (40)	10.4	7.8	5.2	3.7
Kr^+ (84)	11.2	8.4	5.6	3.9
Xe^+ (131)	11.6	8.7	5.8	4.1

Damage

Damage Free

Thus, current silicon industry must replace to new process equipment cyclically with a progress of device miniaturization. But newly developed plasma process equipment completely free from damages has been confirmed to be continuously used to the entire technology node right now. In current semiconductor manufacturing, about 100 plasma processings such as plasma CVD, RIE and sputtering film depositions having severe charge-up damages are used through the entire processings of silicon LSI productions, so that the very severe

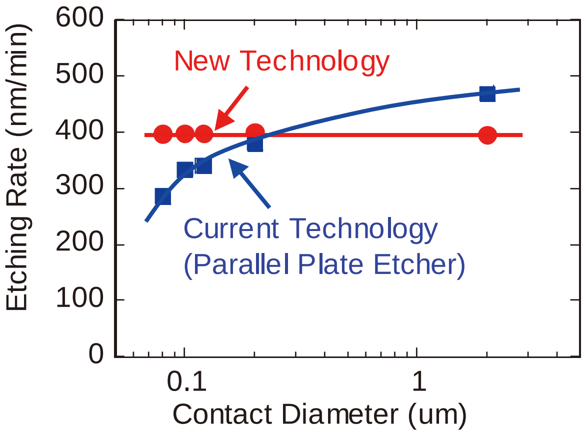


Figure 2 SiO_2 film etching rate dependence on pattern size from 2 um to 80 nm by $Ar/C_5F_8/O_2$.

regulation must be introduced to circuit layout patterns to realize high yield productions where the antenna ratio defined by the gate interconnect total area to the gate electrode area of MOS transistor must be smaller than 100. These regulations to the circuit layout patterns of LSI can be completely eliminated by an introduction of new plasma process equipment completely free from damages(1), so that the performance of silicon LSI will be enhanced drastically.

Furthermore, the gas flow patterns in the process chamber of newly developed plasma equipment are very well regulated by introducing the shower plate structure supplying the plasma excitation gases and the radical generation gases from the upper shower plate and process gases for thin film depositions and pattern etchings from the lower shower plate where the shower plate consists of very many gas injection holes having a diameter of 0.15mm to 0.20mm at the surface of aluminum alloy such as Al Mg (4.5%) Ce (1%) Zr (0.1%) covered with Al_2O_3 passivation films having complete anticorrosion capability and no moisture molecule emissions (4). The total number of gas injection holes is designed that the gas injection speed to the process chamber must be completely smaller than the sound velocity (340m/sec) to maintain the very uniform laminar flow patterns in the process chamber, while the gas flow patterns in the current plasma process equipment are completely different from the uniform laminar flow, i.e., the turbulent gas flow patterns resulting in a huge amount of reaction product adhesion to the inner surface of the process chamber. In the newly developed process chamber having very uniform laminar flow pattern, there does not appear the reaction product adhesion to the inner surface of the process chamber.

Thus, completely new processings will become available, i.e., different thin film continuous depositions in the same process chamber only by changing process gasses and different thin film continuous etchings in the same process chamber only by changing process gases succeedingly. These are completely impossible so far, we are now getting into the new era of manufacturing of semiconductor devices, large size flat panel display and silicon thin film new solar cells where the volume production productivity will be improved very drastically by a factor of at least ten with keeping very high quality process results and improving the device performance drastically, i.e., the realization of the revolutional progress.

2. 915MHz Metal Surfacewave Excitation Plasma

In order to realize completely damage free radical reaction based processing and continuous deposition and etching of multilayer thin films in the same process chamber with changing the process gases, which drastically increase the productivities and

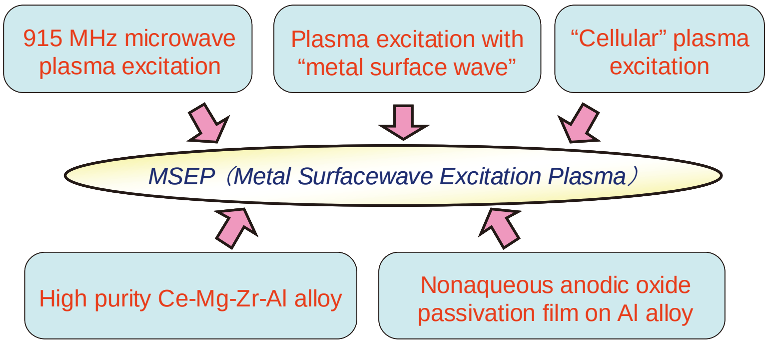


Figure 3 Five key technologies to realize newly developed plasma equipment "MSEP".

reduce the production costs, we have developed a new plasma process quipment collaborating with Tokyo Electron Limited. Five new technologies to realize MSEP are summarized in Fig. 3. The first one is 915 MHz microwave plasma excitation. The electron temperatures of the microwave plasma are generally very low (typically < 1 eV in the diffusion plasma region), since the alternate microwave electric field in the plasma changes before the electrons are accelerated by the microwave electric field and get high kinetic energies. The kinetic energies of the ions incident on the substrate and the chamber walls, which are proportional to the electron temperature as given by Eq. (2), are also kept very low. Therefore MSEP is completely free from plasma-induced damages and metal contaminations from the chamber walls. When the electron density in the plasma is lower than the cutoff density, the incident microwave to the plasma propagates into the plasma. Then, unstable plasma is excited near the substrate. The electron temperature around the substrate becomes high. It is not suitable for the plasma processing. On the other hand, when the electron density is higher than the cutoff density, the incident microwave reflects at the plasma surface. The plasma is excited in the vicinity of the plasma surface by the evanescent electric field. The stable plasma with the low electron temperature can be produced around the substrate. It is applicable for plasma processing. The stable plasma with low electron temperature can be produced only when the electron density at the plasma surface is much higher than the cutoff density over the entire plasma excitation area. In this respect, the cutoff density n_c should be lower, because the stable plasma is produced even at the lower electron densities. Most popular frequency to excite the microwave plasma is 2.45 GHz. At 2.45 GHz, the value of the cutoff density n_c is 7.45×10^{10} cm^{-3}. This value is too high to always produce stable and uniform plasmas for various process conditions. The process window must be much wider to realize continuous deposition and etching of multilayer thin films in the same process chamber. By decreasing the plasma excitation frequency from 2.45 GHz to 915 GHz, the cutoff density n_c becomes about 1/7 (1.04×10^{10} cm^{-3}). Thus, the stable plasma can be excited even at extremely low electron densities and the process window becomes much wider.

We have discovered that the microwave propagates along with the plasma sheath between the metal and the plasma as a TM (transverse magnetic) mode. The width of the plasma sheath is 50~300 μm for the typical process conditions. The power density of the metal surfacewave is extremely high as compared with other propagation types. We have also revealed that the metal surfacewave efficiently excites high-density plasma. By the way, if the wavelength of the surface wave is longer than about 100 mm, it may be difficult to produce the uniform plasma over the entire substrate surface. The free space wavelength of 915 MHz is 328 mm (>100 mm). But fortunately, the wavelength of the metal surfacewave is much shorter than the free space wavelength.

Figure 4 shows the structure of MSEP cell. The dotted lines in Fig. 4(a) are virtual boundaries of the cell. The cell size is 218×218 mm in this case. In the center of the each cell, there is a rectangular metal electrode. A rectangular dielectric plate is inserted between the metal electrode and a large top Al alloy plate. The top plate is also covered with rectangular metal covers. The shape and size of the metal electrode is same as the metal cover. The 915 MHz microwave is fed through the coaxial waveguide in the center of the cell, and radially propagates in the dielectric plate. At the edge of the dielectric plate, the microwave becomes the metal surfacewave and propagates on the metal electrodes and the metal covers covered with Al_2O_3 passivation film. On the metal electrodes and the metal covers, two-dimensional standing waves arise by the interference of the multi-directional metal surfacewaves. The patterns of the standing wave on the metal electrodes and the metal covers are completely same because the shapes and the sizes

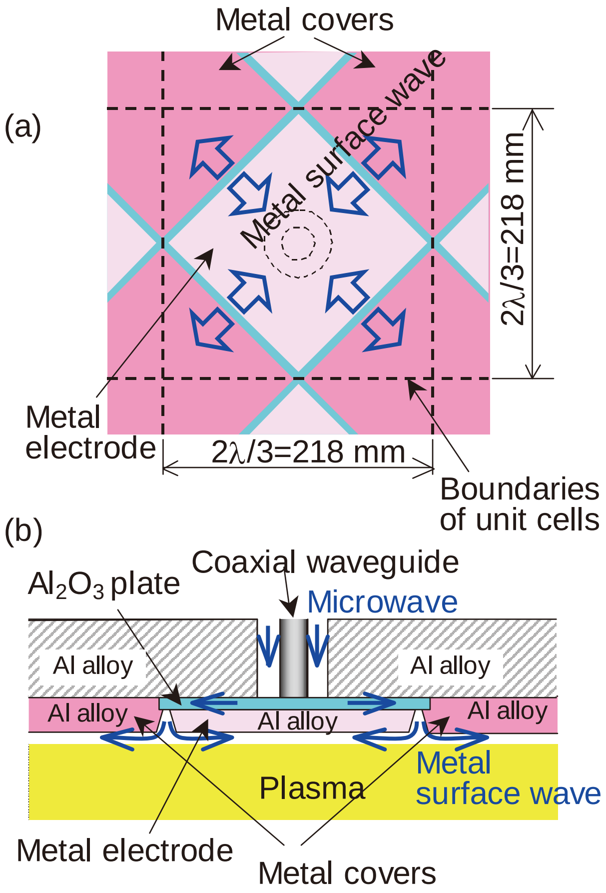
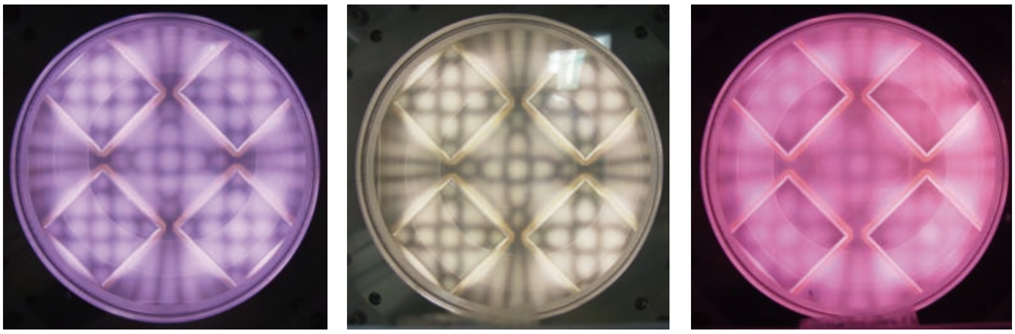


Figure 4 Structure of MSEP cell. (a):bottom view, (b) cross sectional view.

are the same. By this symmetrical structure, the uniform plasma can be excited over a wide range of the process condition. Figure 5 shows the photographs of typical Ar/O_2, O_2 and NF_3 gas ambience plasmas produced in the MSEP equipment. In the MSEP, it can be seen that uniform and stable plasma is excited at relatively low power densities even for 100% O_2 gas ambience and 100% NF_3 gas ambience. We also revealed that the stable plasma without mode jump can be produced over a wide range of electron density from 1×10^{11} to 1×10^{13} cm^{-3}.

Figure 6 shows the cross sectional sketch of the MSEP equipment for semiconductor manufacturing. For the plasma CVD and RIE, both of an upper shower plate and a lower shower plate are settled above the wafer stage. The upper shower plate supplies the plasma excitation gases and the radical generation gases such as Ar, Kr, Xe, O_2, H_2, and NH_3 and etc. The lower shower plate supplies the process gases for deposition or



1.86 W/cm^2 Ar/O_2 (50%)

2.33 W/cm^2 O_2 (100%)

2.33 W/cm^2 NF_3 (100%)

Figure 5 Photographs of Ar/O_2, O_2, and NF_3 plasmas produced in an experimental MSEP equipment. The gas pressure was 67 Pa.

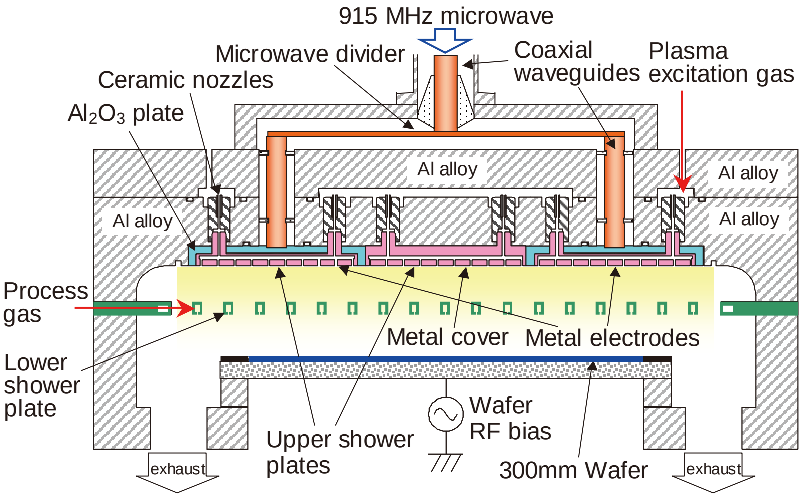


Figure 6 Cross sectional sketch of MSEP for semiconductor manufacturing

etching. The lower shower plate is settled in the diffusion plasma region where the electron temperature is very low. On the other hand, for the radical oxidation, nitridation, oxinitridation, and plasma doping, only upper shower plate is settled. The upper shower plate consists of four metal electrodes and one metal cover, which are regularly arranged on the bottom of the top plate. The 915 MHz microwave fed from the top coaxial waveguide is divided by a microwave divider. The 915 MHz microwave with completely same amplitude and same phase is supplied to four metal electrodes. The microwave propagation lines are carefully designed to minimize the microwave reflections and maximize the plasma excitation efficiency. The chamber, metal electrodes, metal cover, lower shower plate and top plate are made of high purity Ce-Mg-Zr-Al alloy, whose surfaces are covered with nonaqueous anodic oxide passivation film Al_2O_3 with perfect anticorrosion resistance and no moisture molecule emission.

Current high dose ion implantations induce serious charge-up damage in the silicon crystal, because there is little charge compensation mechanism when the huge amount of positive-charged ions are implanted to silicon substrate such as 1×10^{15} cm^{-2} high dose implantation to the source and drain region. Very high electric field intensity larger than 1×10^{5} kV/cm appears in the silicon due to this positive charge, which is enough to induce huge amount of serious damages in silicon crystal. MSEP equipment is quite suitable for realizing very advanced damage free plasma doping technology. 915 MHz MSEP can realize very stable plasma excitation for the gas ambience of 100% PF_3 and BF_3 such as $PF_3 \rightarrow PF_2^+ + F^-$, $BF_3 \rightarrow BF_2^+ + F^-$, where the very high self-bias voltages up to –5 kV and –10 kV can be easily produced on the silicon substrate surface by applying RF power to the substrate electrode without disturbing the plasma with the very effective grounded plane of MSEP. Furthermore, to eliminate charge-up damage completely, high dose doping is divided to $\sim10^{5}$ times doping by introducing pulsed RF application to the substrate electrode. Typical process sequence is shown in Fig. 7, where the pulsed RF bias (pulse width of 10～20 us, duty ratio of 10～20%) is applied to generate the pulsed self-bias voltages of –5～–10 kV. Generated positive charges on the silicon surface are completely cancelled by the electrons flowing from the diffusion plasma region cyclically. Figure 8 shows typical ion implanted profile obtained by simulation, where (a) energy distribution function of BF_2^+ ions subject to the silicon substrate, (b) implanted depth profile of boron, (c) energy distribution function of PF_2^+ ions subject to the silicon substrate, and (d) implanted depth profile of phosphorous as a parameter of frequencies of RF power application from 1 MHz to 10 MHz. In this simulation, 70,000 times –5 keV implantation for determining implanted front and 30,000 times –0.3 keV implantation for maximizing the boron concentration at the silicon surface (larger than 2 $\times 10^{20}$ cm^{-3}) are performed with a total dose of $3\times10^{14}cm^{-2}$. In the case of PF_2^+ ions implantation, 45,000 times –7 keV implantation, 22,000 times –3 keV implantation, and 33,000 times –0.3 keV implantation are performed with total dose of $5\times10^{14}cm^{-2}$. It is revealed that RF frequency of 4～6 MHz is optimum for applying plasma doping. The plasma doping is carried out to the bare silicon surface not the through oxide implantation, so that the annealing temperature can be decreased down to less than 600℃(5).

MSEP is the unique plasma equipment that enables completely damage free radical reaction based processing and continuous deposition and etching of multilayer thin films in the same process chamber only by changing the process gases. The process performances in the radical oxidation, nitridation, oxinitridation, plasma CVD, RIE, and plasma doping will be drastically improved. We plan to produce a lot of MSEP equipments for the volume productions of semiconductors, solar panels, and flat panel displays.

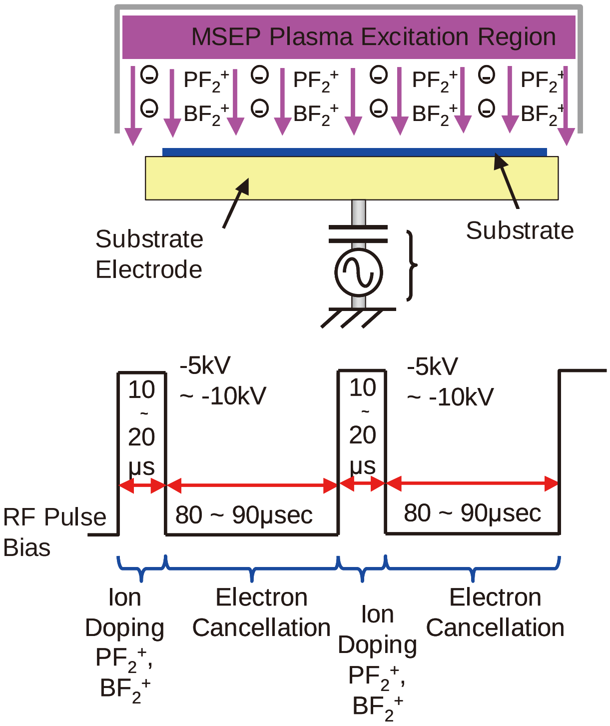


Figure 7 Typical process sequence, where the pulsed RF bias (pulse width of 10～20 us, duty ratio of 10～20%) is applied to generate the pulsed self-bias voltages of -5～-10 kV.

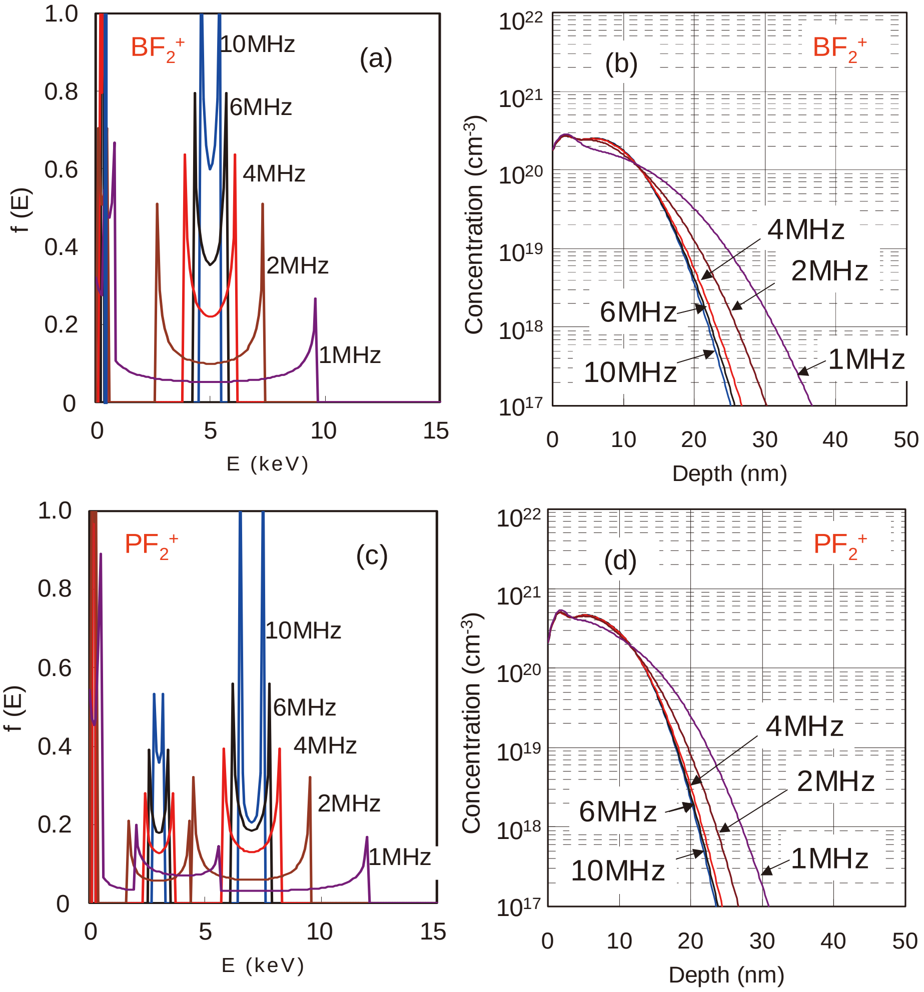


Figure 8 Typical ion implanted profile obtained by simulation, where (a) energy distribution function of BF_2^+ ions subject to the silicon wafer substrate, (b) implanted depth profile of boron, (c) energy distribution function of PF_2^+ ions subject to the silicon wafer substrate, (d) implanted depth profile of phosphorous as a parameter of frequencies of RF power application from 1 MHz to 10 MHz.

3. Al_2O_3 Passivation Films on Aluminum Alloy (AlMg CeZr) Surface

In order to establish very reliable MSEP equipment described in the previous section, Al_2O_3 passivation films having complete anticorrosion resistance and no moisture molecule emissions must be introduced on aluminum alloy surfaces where the high density plasma of various gas ambience such as O_2, H_2, and halogen gases (Cl_2, HCl, HBr, NF_3, BF_3, PF_3 C_5F_8 and etc.) is excited continuously. Al_2O_3 passivation films have been developed on pure aluminum surface and aluminum alloy (AlMgZr) surface by introducing the nonaqueous anodic oxidation using the nonaqueous electrolyte solution (79% ethylene glycol + 20% ultra pure water + 1% ammonium adipate {$H_4NO_2C(CH_2)_4CO_2NH_4$}) (4). The ammonium adipate is unique electrolyte material to obtain electro-conductivity at around pH of 7.0, which is strictly required for the aluminum alloy surface as shown in Fig. 9, where aluminum alloy surfaces are going to be dissolved to the solution having pH value lower than 4.0 and higher than 8.5. The relative dielectric constant of this nonaqueous electrolyte solution is 51, so that the applied voltage can be increased up to 200V without accompanying heterolysis dissociation of H_2O molecules ($H_2O \rightarrow H+OH^-$). The thickness of Al_2O_3 films is limited to 0.3 μ m coming from this applied voltage (4). The nonaqueous anodic oxide Al_2O_3 has been confirmed to exhibit no moisture molecule emission so that the process ambience in the process chamber is maintained completely clean. Newly developed Al_2O_3 films is completely different from conventional aqueous anodic oxidation alumite film which emit huge amount of moisture molecules (4).

In order to increase the passivation film thickness, we have introduced diethylene glycol instead of ethylene glycol so that the nonaqueous electrolyte solution is converted to (79.5% diethylene glycol + 20% ultra pure water + 0.5% ammonium adipate) which relative dielectric constant is decreased down to 44. This newly introduced nonaqueous electrolyte solution exhibits higher viscosity, so that the practical viscosity must be decreased to obtain high quality Al_2O_3 passivation films. We have evaluated two different processings such as to add IPA (Isopropyl alcohol: having a viscosity of 2.3 cp and a relative dielectric constant of 18), and to increase the temperature of the electrolyte solution, as shown in Fig. 10. It becomes very clear from Fig. 10 that the voltage during the constant current mode of $1mA/cm^2$ increases completely linear manner up to 400V only when the electrolyte solution temperature is increased higher than 40℃, so that the temperature of newly introduced diethylene glycol electrolyte solution is maintained at 50℃ for practical productions. Al_2O_3 film thickness can be increased to 0.5 μ m. In order to increase the mechanical strength of aluminum alloy, Mg concentration is increased to 4.5% and additionally 1% Ce is introduced. The anticorrosion capability of aluminum alloy Al_2O_3 passivation films particularly to Cl_2 ambience is enhanced very drastically as shown in Fig. 11, where the weight loss of the aluminum alloy sam-

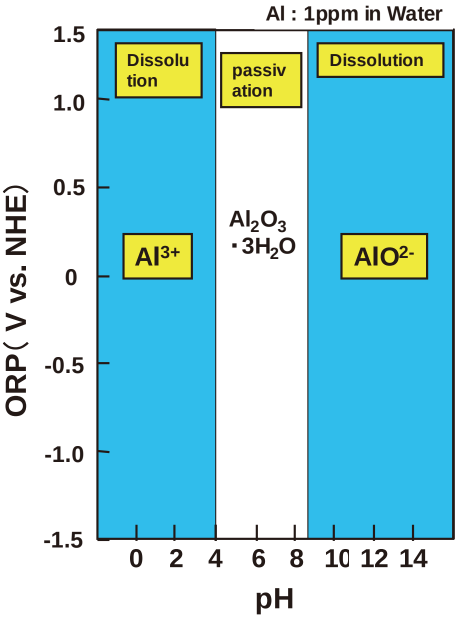


Figure 9 Pourbaix diagram of aluminum

ple covered by Al_2O_3 films is plotted after the Cl_2 ambience exposure test, i.e. the samples are exposed to 100% Cl_2 ambience of 0.3 MPa during 6 hours at 200℃. After the Cl_2 ambience exposure test, the samples are cleaned up by the ultra pure water for 10min. The weight loss due to this high pressure and high temperature 100% Cl_2 ambience exposure test having 0.3 MPa at 200℃ during 6 hours has been confirmed to decrease down to 0.02% from 0.87% by adding 1% Ce to Al 4.5% Mg 0.1% Zr alloy.

Thus, we are now using Al 4.5% Mg 1% Ce 0.1% Zr alloys to the very advanced plasma process equipment, where the standard enthalpy of formation to form oxides is –279 kJ/mol of Al_2O_3, -301kJ/mol of MgO, -299 kJ/mol of Ce_2O_3 and –275kJ/mol of ZrO_2 as shown in Fig. 12, so that we can obtain very high integrity Al_2O_3 passivation film on this aluminum alloy.

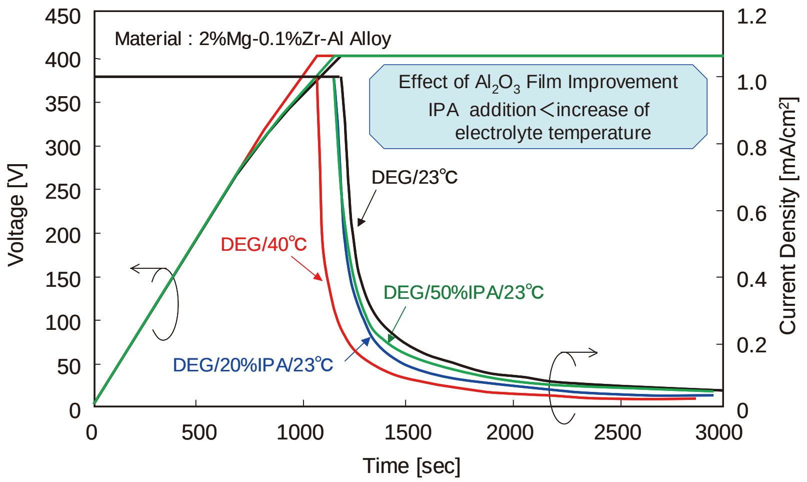


Figure 10 Current voltage characteristics for two different processings such as to add IPA (Isopropyl alcohol: having a viscosity of 2.3 cp and a relative dielectric constant of 18), and to increase the temperature of the electrolyte solution.

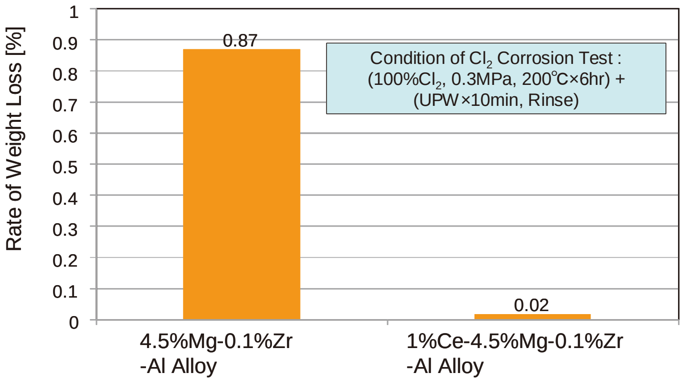


Figure 11 Cl_2 corrosion test results for Al 4.5% Mg 1% Ce 0.1% Zr alloy and Al 1% Ce 4.5% Mg 1% Ce 0.1% Zr alloy.

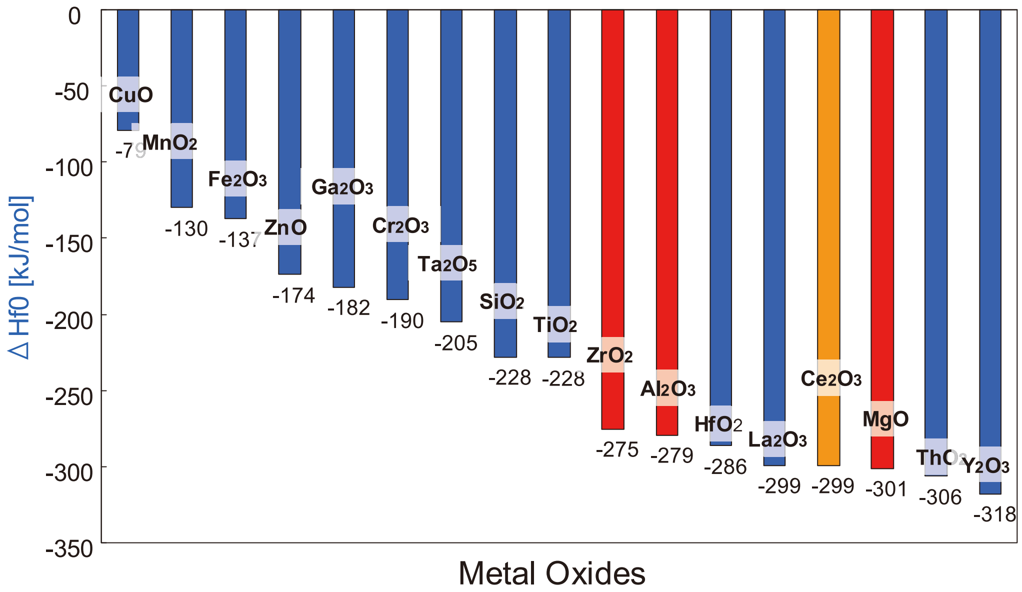


Figure 12 The standard enthalpy of formation to form various metal oxides.

5. Conclusion

We are now establishing science based new silicon technologies by developing radical reaction based semiconductor manufacturing where very high integrity gate insulator films such as SiO_2 and Si_3N_4 can be formed on any crystal orientation silicon surface with the same formation speed, so that silicon LSI will be fabricated on any crystal orientation silicon surface using 3D structure MOS transistors right now, i.e., the entire capability of the silicon crystal can be used to the practical applications. Silicon LSI technologies are going to change very drastically, because the current silicon technologies can fabricate LSI only on the (100) silicon surface using only 2D structure MOS transistors where the relatively high integrity gate insulator film is obtained only on the (100) silicon surface.

Radical reaction based manufacturing essentially requires new plasma process equipment completely free from contaminations and damages, so that we are now developing 915 MHz metal surfacewave excitation plasma (MSEP). MSEP with the single shower plate is used to the radical oxidation, the radical nitridation, the radical oxi-nitridation, and damage free plasma doping instead of current high dose ion implantations giving rise to very severe charge-up damages. MSEP with the dual shower plate is used to the plasma CVD and RIE completely free from damages. Damage free plasma process equipment has been confirmed that the process speed such as etching speed and film deposition speed is completely independent of the pattern size, i.e., this newly developed damage free plasma process equipment has been confirmed to be used to the entire technology node permanently. This is very different from current manufacturing equipment where the process speed decreases with a decrease of the pattern size, so that the current process equipment can be used only two to three technology node, i.e., industries must replace the manufacturing equipment cyclically every two to three technology node by investing huge amount of money.

Furthermore, damage free plasma process equipment has been confirmed to eliminate the regulation of the circuit layout pattern of LSI circuit such as antenna ratio regulation. About 100 plasma processings are used for the entire LSI productions at present, so that the antenna ratio of the circuit layout must be designed less than 100 in order to obtain high yield productions. For the circuit layout patterns including higher antenna ratio larger than 1,000 and 10,000, the production yield is going to degrade with an increase of antenna ratio. Arbitrary free circuit layout patterns can be used by an introduction of damage free plasma process equipment right now, i.e., the very exciting progress of LSI performance.

Gas flow patterns in the process chamber of MSEP covered with Al_2O_3 passivation films having perfect anticorrosion capability and no moisture molecule emission are very well regulated to the very uniform laminar flow pattern by an introduction of very advanced shower plate structures, resulting in no adhesion of reaction products to the inner surface of the process chamber. Thus, very difficult and completely new processings such as different thin film continuous depositions and different thin film continuous etchings in the same process chamber only by changing the process gases continuously will become available, i.e., the revolutional progress of the volume production productivity by a factor of at least ten with keeping very high quality process results and simultaneously improving the performance of silicon LSI for example over 100 GHz clock rate very high speed operations.

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On the structure, properties and applications of metallic glasses

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1 .Introduction

Metallic glasses (MGs), currently on the cutting edge of Materials Science research, are metastable materials that lack the long range order of conventional crystalline metals. Inspite of their non-crystalline structure, the attractive interactions and the size differences between constituting atomic species lead to a short and medium-range order characterized by clusters of atoms which connect to fill the space nearly as densely as their crystalline counterparts [1].

For about two decades after the discovery of the first glassy alloy quenched from the liquid in 1960, the critical cooling rate for suppression of crystallisation was extremely high (of the order of 10^6 K/s), limiting the sample thicknesses to less than 100 μm and impeding their wide application. In the 80's, an improvement of the maximum size of glassy specimens was achieved for a few alloys using fluxing techniques, bringing down the critical cooling rates to about 10^4K/s. However, the trend changed in the early 90's and bulk metallic glasses emerged as an important and promising new class of materials. Since then, a large number of bulk alloys has been quenched to a glassy state with thicknesses reaching several centimeters and critical cooling rates sometimes as low as 1 K/s. This dramatic improvement in the glass formability was related to alloys having three main features, i.e. multi-component systems, significant atomic size differences above 12% between their components and negative heats of mixing [2].

The disordered atomic structure of metallic glasses results in a combination of exceptional mechanical, electrochemical, tribological and soft magnetic properties which are often superior to those of their crystalline counterparts. The combination of their unique properties with their good formability through viscous flow in the supercooled liquid state, and their near-net-shape casting ability has led to several applications as in sensors, magnetic devices, reinforcements for high-performance sports equipment, micromotors, springs, armor devices, biomedical implants and ornaments. However, the field of metallic glasses is believed to possess high potential for further development.

Here we report on the structure, the deformation behavior and some applications of metallic glasses. In section 2.1 we show that binary Zr-Cu binary metallic glass can be approximated as an ideal solution, whereas the addition of Al induces deviations from the ideal solution behavior. In section 2.2 using synchrotron radiation in transmission mode, we report X-ray microprofiling diffraction data of a 30 mm diameter bulk sample prepared at the WPI-AIMR of Tohoku University. In section 3, we report on the temperature rise in the shear bands and the effect of sample size on the deformation mechanism in metallic glasses. In section 4 we propose a new application for metallic glasses; their use as reinforcements for the development of novel light weight composites with high specific strength.

2. Structure

2.1 Detection of deviations from ideal solution behavior in Zr-Cu metallic glasses with addition of Al using synchrotron light

The use of synchrotron light can be highly advantageous for analyzing the structure of metallic glasses [3]. Whereas conventional X-ray beams are completely absorbed near the surface, high energy, high flux radiation penetrates even thick samples, providing a deeper understanding of the unique internal structure of metallic glasses.

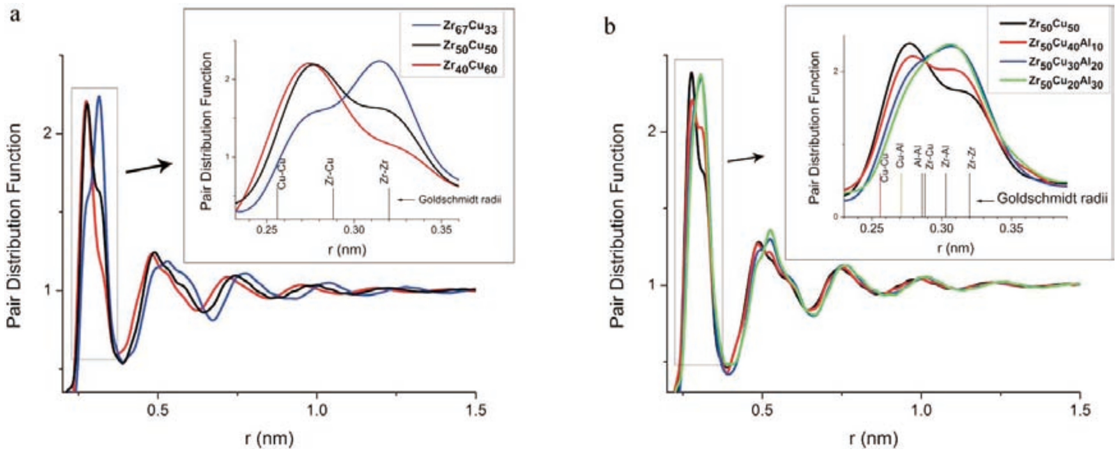


Figure 1: Pair distribution functions for Zr-Cu binary (a) and Zr-Cu-Al ternary (b) metallic glasses. Insets: close-up of the first PDF peak [4].

Using real space pair distribution functions (PDFs) derived from high precision x-ray diffraction data, we attempt to probe the internal structure of metallic glasses based on Zr and Cu and investigate the effect of a third element (Al) in their atomic structure. The results provide a guide for producing thicker glassy alloys with enhanced functionalities.

The PDFs of the Zr-Cu binary metallic glasses (figure 1a) reveal how the atomic structure changes with the Zr/Cu atomic ratio. Increasing Cu content generates significant differences in the PDFs, suggesting modifications in the short (SRO) and medium range order (MRO) up to 1.5 nm. As expected, the structural changes in the nearest neighbor (nn) shell [inset figure 1(a)], indicate an increased number of Zr-Zr atomic bonds for the Zr-rich compositions, and increased number of Cu-Zr and Cu-Cu atomic bonds for the Cu-rich site.

Addition of Al to the Zr-Cu metallic glasses leads to significant modifications of short (SRO) and medium range order (MRO), figure 1b. The nn shell [inset figure 1(b)] indicates the formation of a significant number of Zr-Al atomic bonds. This behavior can be attributed to strongly attractive Zr-Al atomic interactions consistent with the highly negative heat of mixing ΔH_{mix} of -44 kJ/mol which is twice as negative as for Zr-Cu (-23 kJ/mol) whereas ΔH_{mix} for Cu-Al is negligible (-1 kJ/mol). Al has an intermediate atomic size between those of Zr and Cu atoms. Because of the strongly negative heat of mixing between Zr and Al atoms, addition of Al promotes chemical short range ordering in the liquid, improves the local packing efficiency and slows down long range atomic diffusion required for crystallization, leading to increased glass forming ability (GFA).

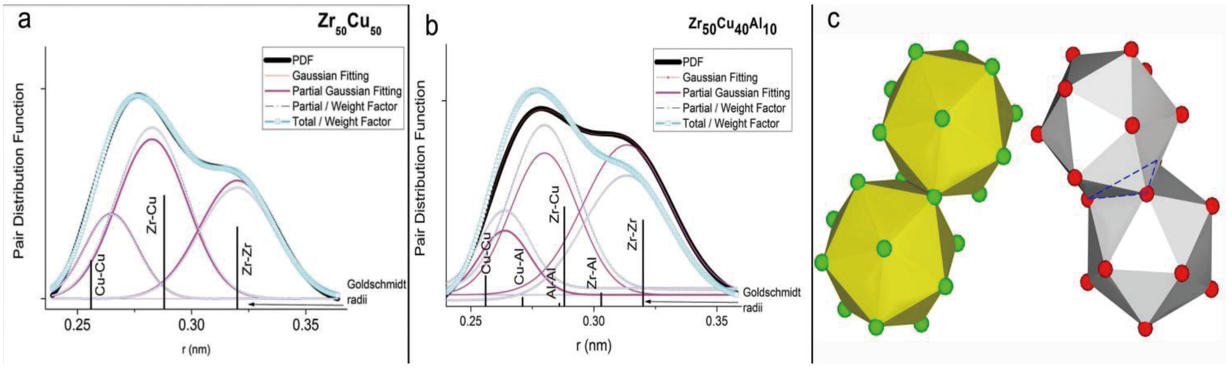


Figure 2: Gaussian fitting of the first PDF peak for a) $Zr_{50}Cu_{50}$ and b) $Zr_{50}Cu_{40}Al_{10}$ metallic glasses. Thick black curves: experimental PDFs, thin red curves: calculated partial PDFs derived from the experimental total PDFs, thin blue discontinuous curves: Gaussian partial PDFs scaled to the weight factors of an ideal solution and thick discontinuous light blue curves: expected total PDFs based on the weight factors [4], c) schematic diagram showing how the atoms in Zr–Cu based metallic glasses form icosahedral clusters that pack tightly together by sharing faces (right) or edges (left) [5].

For an ideal solution, the total pair distribution function (PDF) for Zr-Cu binary alloys would be correlated with the partial PDF of Zr-Zr, Zr-Cu, and Cu-Cu atomic pairs according to the following relation.

$$G(r)=W_{ZrZr}G_{ZrZr}+W_{CuCu}G_{CuCu}+2W_{ZrCu}G_{ZrCu} \quad (1)$$

Approaching the ternary ZrCuAl alloys as ideal solutions, the correlation between total and partial PDFs would be given as following:

$$G(r)=W_{ZrZr}G_{ZrZr}+W_{CuCu}G_{CuCu}+W_{AlAl}G_{AlAl}+2W_{ZrCu}G_{ZrCu}+2W_{ZrAl}G_{ZrAl}+2W_{CuAl}G_{Cu} \quad (2)$$

where $W_{ij}= C_iC_jF_iF_j/(\Sigma\ C_iF_i)^2$, W_{ij} are the ideal solution weight factors, C_i are the atomic concentrations, F_i are the atomic form factors, G(r) are the total PDFs and G_{ij} are the partial PDFs.

The PDFs deriving from experimental XRD results for Zr-Cu binary metallic glasses were found to be in good agreement with those expected from the weight factors of eq (1) (figure 2a), indicating that the Zr–Cu metallic glass can be satisfactorily approximated as an ‘ideal solid solution’. Because of the relatively weak interactions between Zr-Cu atoms in the binary alloy, only thin glasses can be cast from Zr–Cu liquid alloys. However, adding a third strongly interacting component, aluminum (Al), to the liquid alloy leads to a stronger glass that can be cast at thicknesses of up to several millimeters.

We have therefore determined that in contrast to the binary Zr–Cu, ternary Zr–Cu–Al metallic glasses deviate markedly from ideal solution behavior, figure 2b. Zr–Cu–Al liquids and glasses are comprised of finite regions of atomic order, providing the extra resistance to crystallization needed to form thicker glasses. This phenomenon is believed to be due to attractive interactions between the sp-electrons of aluminum and the d-electron shell of the larger zirconium atoms. The atoms arrange in clusters resembling icosahedra, which pack together tightly in the glass (figure 2c), as observed in a previous study [5].

2.2 X-ray diffraction micro-profiling of a 30 mm diameter Zr based BMG from the WPI-AIMR Tohoku University at the European Synchrotron Radiation Facility

A Zr-based bulk metallic glass sample with composition $Zr_{55}Cu_{30}Ni_5Al_{10}$, received from Dr. Y. Yokoyama of the WPI-AIMR Tohoku University was examined by X-ray diffraction in transmission using high-energy synchrotron light at the European Synchrotron Radiation Facility (ESRF). The sample had the shape of a cylindrical rod with 30 mm diameter and 12 mm height. X-ray diffraction micro-profiling was carried out on 0.75 mm thick slices cut along the casting and the radial axes. X-ray diffraction patterns acquired every 100 μm, revealed the amorphous structure of the examined bulk sample as manifested by the successive diffraction halos and the absence of Bragg peaks in the plots of XRD intensity versus the wave vector Q ($Q = 4\pi \sin\theta/\lambda$ where θ is the diffraction angle and λ the wavelength), figure 3b.

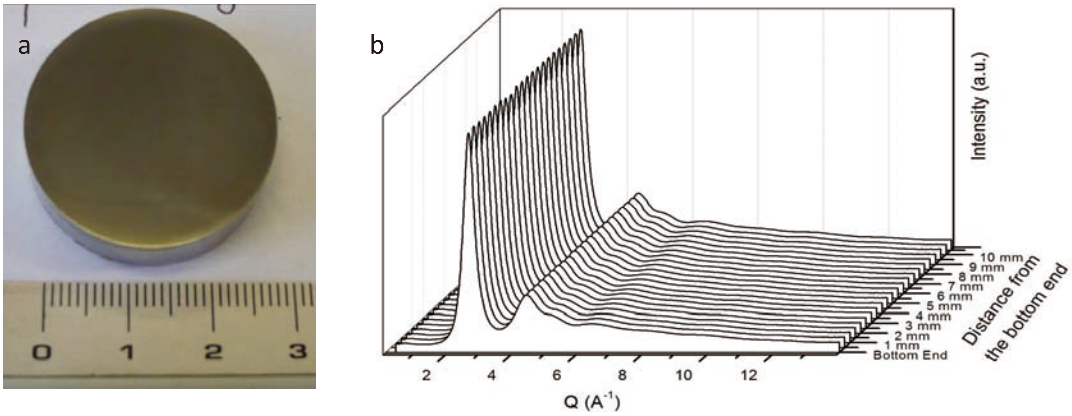


Figure 3: a) Image of the Zr based BMG, b) X-ray diffraction micro-profiling along the cast axis.

3. Size effect on the deformation mechanism of metallic glasses

Metallic glasses exhibit remarkable mechanical properties, such as high mechanical strength up to 5 GPa [6], elasticity up to 2% strain, and good formability through viscous flow in the supercooled liquid state. However, their limited ductility at ambient temperature, especially in tension, serves as a major impediment to their wider application. This behavior is attributed to work-softening and inhomogeneous flow localized in shear bands.

We have recently shown clear and direct evidence of melting in the shear bands in some bulk metallic glasses due to elastic energy release in the form of heat in the shear zones. Shear steps were found at several instances to have been formed in successive increments with evident wear and tear on a thickness scale larger than the expected thickness of about 10 nm for the shear band itself (figure 4). The estimated range of attained temperatures and the observed morphologies are consistent with shear steps forming at a subsonic speed limited by a required redistribution of local microscopic stresses. Calculations indicated that a 0.2 μm thick layer melts in the vicinity of a shear band forming a shear step of the order of 1 μm [7].

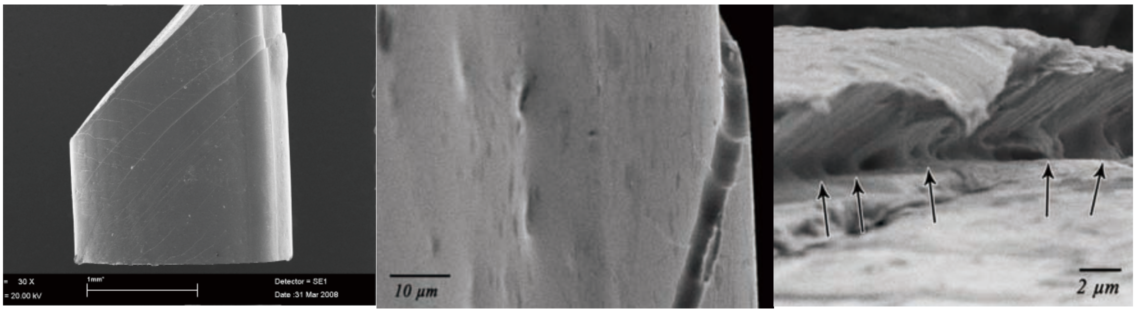


Figure 4: a) SEM images of shear steps formed on the surface of a Zr-based BMG, b) a rather featureless step having formed meniscus with the upper part of the specimen indicating that the entire width of the step of about 5 μm melted at some point, c) arrows show U-shaped meniscus locations at the step bottom indicating viscous behavior and high temperatures at the end of the shear event. [7].

However, below a critical sample size, the temperature rise in the shear bands would be expected to be insignificant. In addition, a scientifically interesting and technologically attractive discovery has been made recently, reporting a transition from inhomogeneous deformation and shear banding to a homogenous deformation mode when the sample size is reduced to below 400 nm [8].

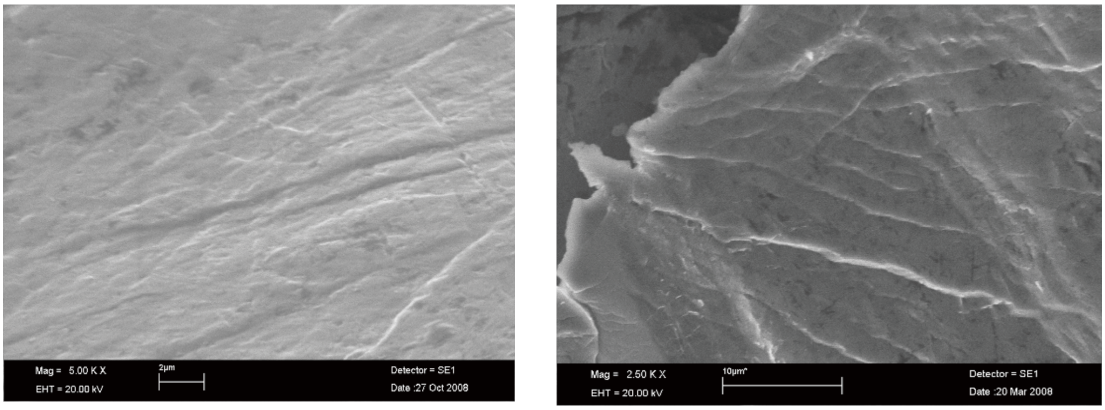


Figure 5: SEM images of the surface of heavily deformed Zr-based metallic glasses [9].

Using a special “soft” ball milling technique, we heavily deformed metallic glass ribbons and obtained foil specimens with thickness in the range of 200 nm to 2 μm. The SEM images of figure 5 correspond to Zr based metallic glasses after such heavy deformation with thickness of the order of 1-2 μm. On the surface of these samples, shear steps can easily be observed, indicating that deformation was carried out by shear banding, in an inhomogeneous deformation mode.

On the other hand, with the decrease of the samples size to thicknesses of the order of 250-300 nm, shear steps disappear from the surfaces of the heavily deformed samples (figure 6), indicating that deformation in these ultra-thin samples was no longer by shear banding, but by a homogenous deformation mechanism. This sample-size induced transition in the deformation mode may be attributed to a critical strained volume necessary to reach sufficiently high energies for the formation of a shear band [8].

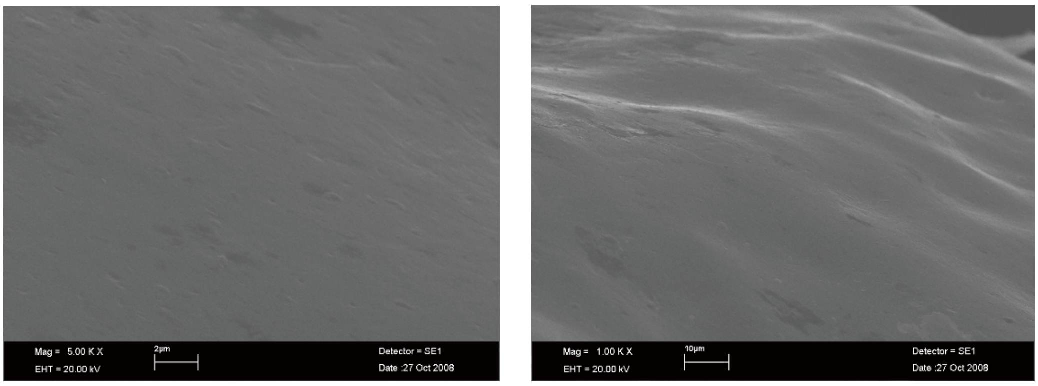


Figure 6: SEM images of the surface of a deformed Zr-based metallic glass with thickness of the order of 250-300 nm [7].

Transmission electron microscopy (TEM) revealed the presence of shear bands in heavily deformed Pd-based metallic glass samples with thickness in the range of 0.5-1 μm (figure 7), indicating that the predominant deformation mechanism is still localized flow and shear banding, as expected for metallic glasses with dimensions above 400-500 nm. The thickness of the observed shear bands is of the order of 20-25 nm.

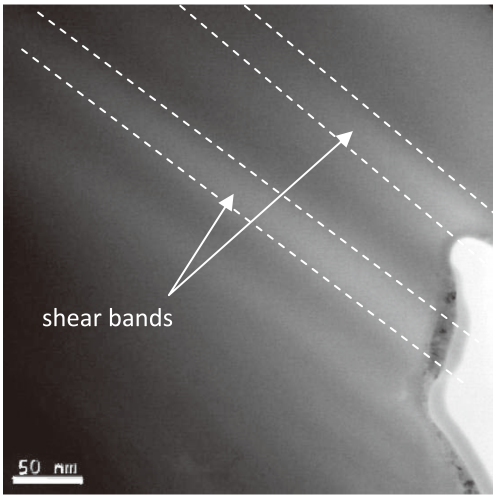


Figure 7: TEM image of a heavily deformed Zr-based metallic glass with thickness around 1μm.

TEM examination of a Zr based metallic glass with thickness of about 250-300 nm after heavy deformation revealed only a homogenous structure, without any evidence for the existence of shear bands (figure 8). This observation indicates that during "soft" ball milling, the thickness of the sample becomes small enough (below 400 nm) to allowed a transition from heterogeneous deformation and shear banding (which is the expected deformation mechanism of metallic glasses at temperatures well below their glass transition) to homogeneous deformation. The above observations seem to be in good agreement with the SEM observations of figures 5 and 6 [9].

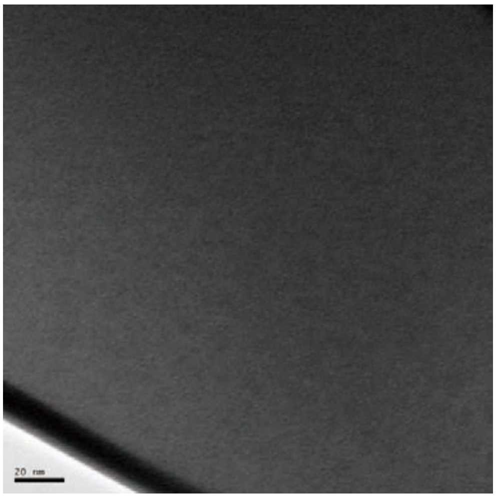


Figure 8: TEM image of a heavily deformed Zr-based metallic glass with thickness below 300 nm.

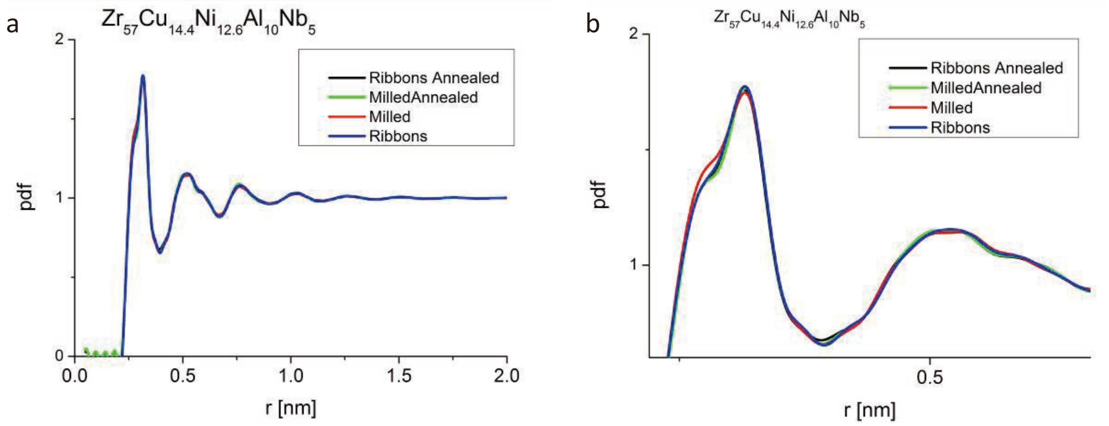


Figure 9: a) Pair distribution functions (PDFs) of metallic glass in the non-deformed and deformed state, b) close-up in the first and second nearest neighbour (nn) shell [9].

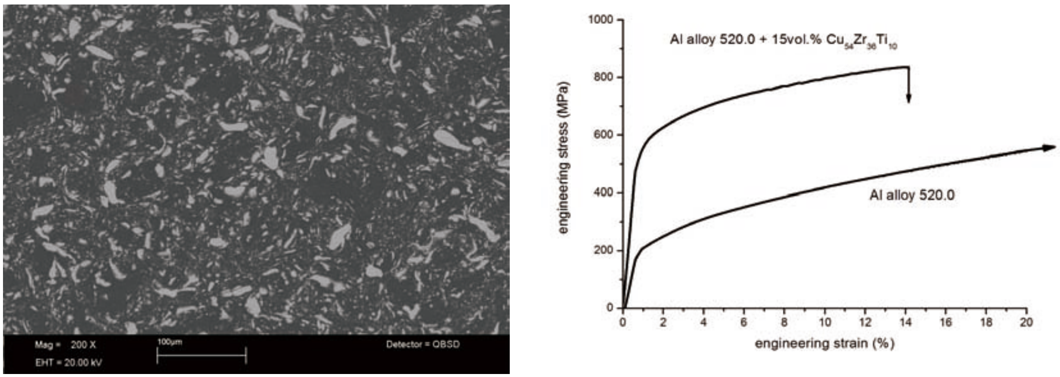
The effect of deformation on the atomic structure of metallic glasses was studied using real space pair distribution functions (PDFs) derived from high precision x-ray diffraction data acquired at the European Synchrotron Radiation Facility (ESRF). Figure 9 shows the pair distribution function of a Zr based metallic glass in the as cast (ribbons) deformed (milled) and annealed state (Ribbons Annealed and Milled Annealed, annealing performed at temperatures between glass transition T_g and crystallization temperatures T_x). No significant changes can be observed in the PDFs between the deformed and non-deformed state (figure 9b). However, a close up of the first and second PDF peak (right figures below) reveals some small differences between the deformed and non-deformed state in the first and second nearest neighbour's shell. This indicates small modifications in the short and medium range order of the atomic structure of metallic glasses induced by heavy deformation. Since we showed earlier that shear banding can result in significant local heating, it is likely that the similarity in atomic structure of the deformed and undeformed metallic glass is due to fast re-establishment of any local (SRO or MRO) atomic order perturbed by the deformation.

4. Some applications of metallic glasses

In addition to the other reported applications of metallic glasses, metallic glasses can also be used as efficient reinforcements in light weight composites with high specific strength, as recently demonstrated [10, 11].

Light-weight materials of advanced performance are now experiencing global interest due to the growing importance of environmental issues and energy saving strategies in land and air transportation and machinery industries. We have recently developed novel light weight composites with improved engineering properties using commercial grade light alloy metal matrices with micro and nanometer scale metallic glass particles as reinforcements. The metallic glass particle dispersions serve both as binder and as reinforcement in Mg-based and Al-based industrial alloys, resulting in composites with full density and good mechanical properties. This novelty uses advantageously the unique property of metallic glass particles to become very soft above their glass transition temperatures (T_g) allowing them to act as a soft binder phase and remove porosity during hot compaction together with light alloy powders. After compaction to full density (fig. 4a) and cooling to below T_g and down to room temperature, the same glassy particles become the hard reinforcement phase due to their 2% elastic strain range, resulting in composite materials with significantly improved strength.

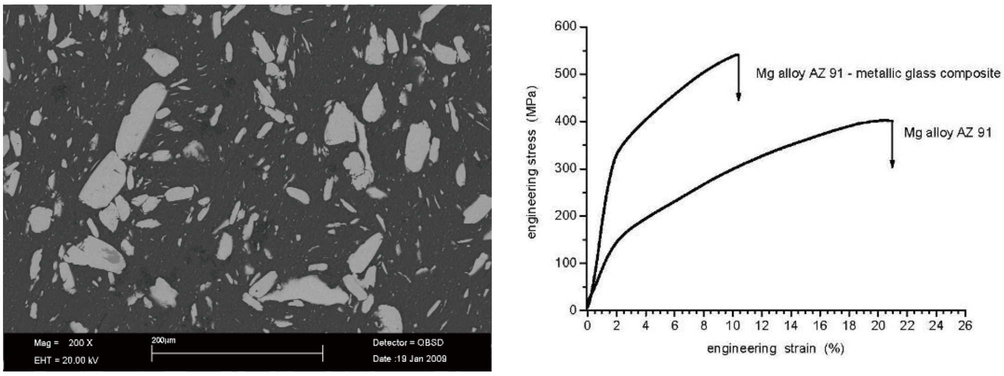
The microstructure of an Al alloy composite reinforced with Cu based metallic glass particles is shown in figure 10a. The bright particles in the back-scattered electron SEM image correspond to the metallic glass phase. The distribution of the glassy particles in the matrix is uniform without any preferred orientation and without any visible pores in the matrix, indicating successful full densification of the composite. Though, a few % of metallic glass particles are still quite large (about 40 μm in one dimension), a significant fraction of the particles is in the range from a few hundred nanometers to 10 μm.



a **b**

Figure 10: a) Microstructure of a novel light weight composite with Al-based matrix and Cu-based metallic glass reinforcement, b) Compression stress-strain curves of the same composite material in comparison with the matrix Al alloy [10].

The yield strength of the Al alloy/ metallic glass composite is about three times higher than that of the matrix alloy. In addition the composite exhibits a mechanical strength at fracture of about 840 MPa and an appreciable plastic strain before fracture of about 13% (figure 10b). This combination of mechanical properties is remarkable and among the best ever reported for an aluminum alloy matrix composite. Furthermore, the results are fascinating in the sense that the composite sintered from powders is much stronger than the matrix alloy produced by casting. This is a reliable indication of successful sintering that produced excellent bonding between the powder particles of the matrix as well as between the matrix and the metallic glass reinforcement particles [10].



a **b**

Figure11: a) Microstructure of a novel light weight composite with Mg-based matrix and Zr-based metallic glass reinforcement, b) Compression stress-strain curves of the same composite material in comparison with the matrix Mg alloy [11].

Similarly, composites with a Mg alloy matrix and a Zr-based metallic glass were also developed recently [11]. The mechanical strength of the composite is markedly increased compared to the Mg alloy, retaining a plastic strain before fracture of about 10%, leading again to a noticeable combination of mechanical properties which is among the best reported for magnesium alloy matrix composites.

5. Summary

Binary Zr-Cu binary metallic glass can be satisfactorily approximated as an ideal solution, due to weak interactions between Zr-Cu atoms. However, adding a third strongly interacting component, aluminum (Al), to the liquid alloy leads to strong deviations from the ideal solution behavior and to a stronger glass that can be cast at thicknesses of up to several millimeters.

SEM observations of shear steps on deformed BMGs show direct evidence of melting as expected from elastic energy release in form of heat during shear deformation. A scientifically interesting and technologically attractive transition from heterogeneous deformation localized in shear bands to a homogeneous deformation mode occurs with reducing samples size down to the 100 nanometer scale. Submicron thickness samples can be produced by a special “soft” ball milling technique.

Micron and submicron metallic glass particles can be used as reinforcements in Mg alloy based and Al alloy based composites producing light weight materials with superior mechanical performance, and thus attractive for energy saving applications in the transportation, aviation and heavy machinery industries.

Acknowledgements

The authors are grateful to Prof. W. Botta of UFSCar, Brazil, for providing TEM facilities and fruitful discussions and to Dr G. Vaughan and the ESRF for synchrotron beamtime and precious advice. This work was done in collaboration with Professor A. Inoue of Tohoku University and Prof. D. Louzguine of the WPI-AIMR.

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2005-present	Associate Bioengineer, Brigham and Women’s Hospital, USA
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2009-present	Junior Principal Investigator, WPI Advanced Institute for Materials Research, Tohoku University

RECOGNITION:

- ✦MIT's Outstanding Undergraduate Research Mentor (2003-2004)
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- ✦Biomedical Engineering Society Outstanding Graduate Student Award (2005)
- ✦OMNOVA/MIT PPST Award - Outstanding Polymer-related Research (2004-2005)
- ✦Coulter Foundation Young Investigator Award in Bioengineering (2006)
- ✦TR35 Top Young Innovator Award, Technology Review (2007)
- ✦BMW Scientific Award (2007)
- ✦Victor K. LaMer Award, Surface and Colloid Science Division, American Chemical Society (2008)
- ✦ IEEE EMBS Early Career Achievement Award (2008)
- ✦ NSF CAREER Award (2009)
- ✦ International Academy of Medical and Biological Engineering Young Faculty Member Award (2009)

CURRENT RESEARCH:

Broadly described, my research involves the merger of microfabrication techniques and advanced biomaterials for generation of engineering systems that can be of benefit for biological and biomedical applications. This is based on developing micro- and nanoscale technologies to control cellular behavior with particular emphasis in developing microscale biomaterials and engineering systems for tissue engineering. We have made a number of important contributions in developing technologies to control the formation of vascularized tissues with appropriate microarchitectures as well as regulating stem cell differentiation within microengineered systems. At Tohoku University my lab will focus on developing microfluidic system that can be used for disease diagnostics as well as engineering of biomaterials that can be integrated into these systems to enhance functionality.

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2001-2006	Assistant Professor, Texas A&M University, College Station (TAMU), USA
2003-present	Director of Center for Nanoscale Science and Technology (CNST), TAMU, USA
2004-present	Joint Assistant Professor, Electrical and Computer Engineering, TAMU, USA
2006-present	Associate Professor, Physics & Joint Ass. Professor, Electrical and Computer Engineering, TAMU, USA
2008-present	Chair of the Faculty Senate Research Committee, TAMU, USA
2009-present	Junior Principal Investigator, WPI Advanced Institute for Materials Research, Tohoku University

RECOGNITION:

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✦ European Union/Science and Technology Agency, Japan Post-Doc Fellow (1998-1999), declined
✦ Montague/Center for Teaching Excellence Scholar, Texas A&M University (2004)

CURRENT RESEARCH:

- Biophysics: Biomolecular Motility and Adsorption Studies
- Nanomagnetism: Single Molecule Magnets
- Highly Correlated Materials: Metal-Insulator Transition in disordered Electronic Systems

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- ✦ Guo Moruo Prize, University of Sci.&Tech. of China (1995)
- ✦ Tsinghua “Hundred Talents” award (2005)
- ✦ Li Foundation Heritage Prize (2006-2007)
- ✦ DuPont Young Professor Grant (2007-2009)

CURRENT RESEARCH:

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WPI-AIMR

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PROFESSIONAL EXPERIENCE:

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RECOGNITION:

✦Daicel Chemical Industries Award in Synthetic Organic Chemistry, Japan (1995)
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CURRENT RESEARCH:

My current research is focused on the development of new nanostructured metals, such as supported metal nanoparticles and nanoporous metals, as heterogeneous metal catalysts for synthesis of functional organic materials.

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2007-2009	Postdoctoral Fellow, Material Research Laboratory, University of California at Santa Barbara 2009-presentResearch Associate, WPI-Advanced Institute for Materials Research, Tohoku University

CURRENT RESEARCH:

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- Multiscale computational study on biological and soft condensed materials

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CURRENT RESEARCH:

- Further development of Atomic Force Acoustic Microscopy (AFAM) and application to engineering and biological materials, i.e. measurement of elastic / visco-elastic properties and investigation of internal friction
- Elastic / anelastic and mechanical properties of Bulk Metallic Glasses

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2004	B.E. in Applied Physics, Tohoku University
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- Study on clathrate materials, high-T_c cuprate superconductors

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2006	Dr. in Materials Science, Institute of Metal Research, Chinese Academy of Sciences, P.R.China

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2006-2008	Assistant Professor, Institute of Metal Research, Chinese Academy of Sciences, P.R.China
2008-2009	Postdoctoral Fellow, National Institute for Materials Science
2009-present	Research Associate, WPI Advanced Institute for Materials Research, Tohoku University

CURRENT RESEARCH:

- Crystallization of Multicomponent Bulk Metallic Glasses

WPI-IFCAM

WPI-IFCAM

International Frontier Center for Advanced Materials (IFCAM) was inaugurated in Institute for Materials Research (IMR), Tohoku University, in October 2001 to function, simply stated, as the world-first "materials science think-tank." With wise steering by past directors, IFCAM has been performing well in its mission until now by 1) bringing in many world-renown researchers to IMR in the greater field of materials science/engineering, 2) enlightening / encouraging young scientists, post-doctoral fellows and graduate students by organizing and supporting workshops/summer schools, and 3) establishing and coordinating IFCAM branch offices around the world, including those in Cambridge University, Harvard University, Stanford University, and Institute of Physics, P.R. China.

We were also so fortunate to have had a government initial-equipment fund in 2002 to acquire several advanced tools, such as 3-dimention atom-probe tomography (3-D AP) and low energy electron microscope (LEEM). With untiring effort of able faculty members and their staff / graduate students, the LEEM program of IFCAM, for instance, has quickly become one of the most active and successful research centers in the world.

Realizing that IFCAM and newly established WPI-AIMR have essentially the same mission: namely, further promote international collaboration and cooperation in innovative research on advanced materials on a global bases, IFCAM was transferred from IMR to WPI-AIMR, effective of April 2008.

Briefly stated, WPI-IFCAM has following function and service.

1. Visiting Professorship
2. Workshops / summer schools

Ⅰ. Visiting Professorship

Qualified researchers who may be interested in IFCAM visiting professorship should first contact the WPI principal investigator(s) of the related research fields. Your contact PIs will initiate the further process to materialize the joint research.

(1) Tenure: For a period of minimum one month to a maximum of 3 months.

(2) Financial: The salary varies, depending on the qualifications, based on the Tohoku University regulations. Roughly speaking, "full professor" receives Y600,000 per month and "Associate Professor" receives Y500,000 per month.

Ⅱ. Workshops / summer schools

WPI-IFCAM will financially support the workshops and summer schools, if the scientific aims are along the WPI-AIMR missions. For more information, please contact WPI Administrative Office.

2009-2010 WPI-IFCAM VISITING SCHOLARS

	Candidate	Host	Position	Term							Term	Affiliation	Position	Graduated from	Diploma	Nationality	Age	Research Proposal
				From			～	Through										
1	**CHALLAPALLI, Suryanarayana**	A. Inoue	Visiting Professor	H21	4	13	～	H21	7	12	3m	University of Central Florida	Professor	Banaras Hindu University, India	Ph. D	USA	64	Synthesis, Processing, and Characterization of Nanomaterials and Bulk Metallic Glasses
2	**LEE, Seung-Hun**	K. Yamada	Visiting Professor	H21	5	28	～	H21	7	15	1m18d	University of Virginia	Professor	Johns Hopkins University, USA	Ph. D	South Korea	45	Novel quantum phenomena in complex transition metal oxides
3	**TEIZER, Winfried**	T. Adschiri	Visiting Associate Professor	H21	6	1	～	H21	8	31	3m	Texas A&M University	Associate Professor	University of Massachusetts, USA	Ph. D	Austria	38	Biophysical applications of magnetic nanoparticles
4	**JIA, Jinfeng**	M. Chen & T. Hashizume	Visiting Professor	H21	7	6	～	H21	10	5	3m	Tsinghua University	Professor	Peking University, P.R. China	Ph. D	P.R. China	43	Growth mechanism of Pb film by LEEM and LTSTM
5	**WANG, Weihua**	M. Chen & A. Inoue	Visiting Professor	H21	8	5	～	H21	10	30	2m26d	Institute of Physics, Chinese Academy of Sciences	Professor	Institute of Physics, Chinese Academy of Sciences, P.R.China	Ph. D	P.R. China	46	Understanding of deformation mechanism of bulk metallic glasses
6	**ORESHKIN, Andrei Ivanovich**	T. Hashizume	Visiting Professor	H21	9	4	～	H21	12	3	3m	Moscow State University	Senior Researcher	Moscow State University	Ph. D	Russia	42	
7	**CHEN, Ho Sou**	A. Inoue	Visiting Professor	H21	10	1	～	H21	11	30	2m	Bell Laboratories, Lucent Technologies	Adviser	Harvard University, USA	Ph. D	USA	76	Development of mechanical properties by fundamental approaches of fragility and relaxation control in metallic glasses.

WPI Activity Report of Professor W. H. Wang
Aug. 5th, 2009- Oct 30th, 2009
Host: Professor M. W. Chen

Two objectives were achieved during this short period of three months at WPI-AIMR in Tohoku University. The first was investigating the role of microalloying on the glass-forming ability and mechanical and physical properties of bulk metallic glasses. Minor addition or microalloying technique, which has been widely used in other metallurgical fields, plays effective and important roles in formation, crystallization, thermal stability and property improvement of bulk metallic glasses. This simple approach can induce giant properties changes in metallic glasses and provides a powerful tool for the BMG-forming alloys development and design. However, up to know, little work has been done on the atomic and electronic origins for the microalloying effect on the properties of the glass-forming alloys. We try here to understand the roles of the minor addition in the formation and the properties of the BMGs and the BMG-based composites by using atom probe technique and simulation. Some interesting data were obtained and a manuscript entitled “Giant properties changes in metallic glasses induced by microalloying” is in preparation.

Another study started was to investigate the correlation between the plastic deformation and relaxation in metallic glasses. Primary work shows that the deformation unit of shear transformation zone (STZ) has close correlation with slow Beta-relaxation in metallic glasses. The study could provide insight on the plastic deformation mechanism and of the metallic glasses, on the other hand, This result has significance for revealing the origin of the beta relaxation in metallic glasses. Work is going on this aspect and it will be continued in future cooperation with Prof. Chen’s group in WPI.

I would like to thanks Prof. Ming Wei Chen and WPI for offering me the opportunity to visit here. The administrative help and support provided by Ms. Mariko Onodera and Ms. Saitoh, and member in Prof. Chen’s group is greatly appreciated.

WPI Activity Report of Professor A.I. Oreshkin
September 4th, 2009- December 3th, 2009
Host: Professor Tomihiro HASHIZUME

Self-organized nanostructures and thin films of organic materials compatible with Si-based semiconductor systems are currently of great interest for expanding microelectronic technologies to nanoscale range and for applications in optoelectronic devices. Among them, carbon fullerenes and their derivatives are very promising for the fabrication of electro-active elements in photovoltaic solar cells, active layers in organic field-effect transistors, and as building blocks for chemical manipulation in nano-science applications to develop new functionalities. During my stay at WPI-AIMR in Tohoku University I was working on project: "The initial adsorption of single $C_{60}F_{18}$ molecules on Si(100)-2×1 surface." In contrast to $C_{60}F_{46\div48}$ molecules (which have been studied before) tortoise-shaped polar (> 9 Debye!) $C_{60}F_{18}$ molecules are very asymmetrical: all the 18 fluorine atoms are bound to one hemisphere of C_{60} only and flatten its shape. It has been found that the all $C_{60}F_{18}$ molecules are very stable and do not react with the surface at room temperature. The step edges and terraces are adsorption sites of equal priority. Being deposited on Si(100)-2×1 surface $C_{60}F_{18}$ molecules occupied the troughs between dimmer rows. High resolution STM images of individual molecule and theoretical calculations of adsorption energy allowed us getting conclusion about possible orientation of $C_{60}F_{18}$ molecule with regard to substrate. The adsorption energy of the molecule, E_{ad} is calculated from $E_{ad} = E(C_{60}F_{18}) + E(\mathrm{Si}) - E(C_{60}F_{18}/\mathrm{Si})$, where $E(C_{60}F_{18})$, $E(\mathrm{Si})$, and $E(C_{60}F_{18}/\mathrm{Si})$ are the total energies of a free $C_{60}F_{18}$ molecule, Si(100)-2×1 surface, and the combined system, respectively. Among the three different orientations of a $C_{60}F_{18}$ molecule considered on Si(100)-2×1 surface, the adsorption energy for the bottom orientation is very high as compared to for the top and for the side orientations. Accordingly it is expected that $C_{60}F_{18}$ molecule would instantaneously align to the bottom orientation, with the fluorine atoms pointing towards the Si substrate. In the mean time our experimental results show that the $C_{60}F_{18}$ molecule always tilted with regard to Si(100)-2×1 surface. Attractive electrostatic interactions between the strongly polarized $C_{60}F_{18}$ molecules probably account for the closeness of the molecules. Step by step annealing of up to 500° C has not revealed any changes in molecular structure. At 500° C molecule starts to decompose. It has been found that in the presence of C-defects on the Si(100)-2×1 surface, they work as attractive centers for $C_{60}F_{18}$ molecules. The manuscript is under the preparation.

I would like to emphasize that I have found an enjoyable and stimulating scientific environment in the WPI-AIMR and I would like to thank the direction of WPI-AIMR and Tohoku University for giving me opportunity to work here. I am very grateful for their kindness and hospitality during my stay in Sendai.

Professor Ho S Chen, WPI Activity Report
October 1, 2009 – November 30, 2009
Host: Professor Akihisa Inoue

The author has conducted series of investigations on the relaxation dynamics of metallic glasses since the early development in 1970's and 1980's. Calorimetric and mechanical dynamic measurements of glassy alloys revealed the sort of secondary relaxation, or beta-relaxation, clearly for many ternary alloys but is nearly absent in binary alloys. In mechanical dynamic relaxation measurements, at f ~ 1 Hz, beta – relaxation loss peak appears, and being well separated from the primary alpha – relaxation at T well below Tg (T ~ ¾ Tg) for many BMG. The most and significant observation is the appearance of two relaxation loss peaks, called sub Tg- and primary Tg – relaxations. The sub Tg- relaxation appears as a shoulder to the Tg – alpha-relaxation peak, while the alpha peak is very narrow and can be fitted fairly well with Debye peak.

Recently, there have renewed interest on the studies of mechanical and structural relaxations of BMG. Two major issues emerge regarding the secondary relaxation and primary relaxation at Tg. Firstly whether all glass forming liquids show high frequency dynamic modes of Johari-Goldstein (J-G) relaxation distinct from the primary alpha relaxations. Secondly the so-called slow beta-relaxation, or excess wing (EW) is just the low free energy tail of the activation barrier distribution of primary alpha-relaxation, and whether the secondary relaxation connected with fragility of BMG.

For past month or so, we critically examined the calorimetric and mechanical dynamic relaxations of classic BMG, Pt-Ni-P, Pd-Ni-P and Pd-Cu-Si alloy glasses. These three glasses belong to rather fragile glasses of m ~ 50 – 60. We find a distinct difference regarding the occurrence of beta- relaxation between Pd-Cu-Si, and Pa-Ni-P and Pt-Ni-P glasses. In all three glasses, there appears distinct beta – relaxation in as quenched samples. However after reheating the samples to Tg, the beta-relaxation disappears in Pd-Ni-P and Pt-Ni-P glass but Pd-Cu-Si glass. Clearly the beta-relaxation in BMG may correlate to fragility as has been proposed by many researchers, but may be not the dominant factor. We suggest that it is the medium-range topological ordering of the glass structure influences greatly the secondary relaxation in BMG.

We also have initiated investigation on the two-step relaxation processes at Tg. We hope that these studies will shade-light better understanding of glass transition of BMG.

Announcement

Announcement
The 2010 WPI-AIMR Annual Workshop

March 25, Thursday - March 27, Saturday, 2010
Sendai Excel Hotel Tokyu and Sendai International Center

http://www.wpi-aimr.tohoku.ac.jp/workshop/

In the process of realizing three major goals of WPI Advanced Institute for Materials Research (WPI-AIMR) of Tohoku University; (1) Invent and develop new and innovative functional materials, (2) Establish a system adequate as a World Premier Research Center, and (3) Strengthen international cooperation and construct a world visible center,
http://www.wpi-aimr.tohoku.ac.jp/en/modules/wraps/index.php/greetings/message2.html,
we have been organizing WPI-AIMR Annual Workshops. Following the 2009 Workshop held on March 1, Sunday, through 6, Friday, 2009, at Miyagi-Zao Royal Hotel, we are announcing the 2010 WPI-AIMR Annual Workshop which will be held on March 25, Thursday, through March 27, Saturday, 2010, at Sendai Excel Hotel Tokyu and Sendai International Center. In the afternoon of March 26, Friday, we plan to have a special session, inviting Professor Thaddeus B. Massalski of Carnegie Mellon University, and also an Executive Secretary of Acta Materialia, Inc., Professor Akihisa Inoue, President of Tohoku University, and Dr. Chikara Hayashi, Chair of Ulvac, Inc. for celebrating Professor Inoue's 2010 Acta Materialia Gold Medal Award;
http://www.materialsaustralia.com.au/scripts/cgiip.exe/WService=MA/ccms.r?PageId=20071.
In the afternoon of March 25 and on March 26 and 27, we will have plenary sessions and parallel sessions including invited presentations by world premier researchers of the four fields of WPI-AIMR research (thrusts), which are Bulk Metallic Glasses (BMG), Nanophysics, NanoChemBio and Device/Systems;
http://www.wpi-aimr.tohoku.ac.jp/en/modules/wraps/index.php/outline/organization/management_system.html.

In the parallel sessions, we highlight current and forthcoming Fusion Researches and sessions of (1) BMG and Nanophysics, (2) Nanophysics, Nonochemistry and Device/System, and (3) NanoChemBio will be arranged. For encouraging younger researchers and further discussing the Fusion Researches, we have a poster session on March 26.

We would appreciate very much if you could join the Workshop.

Tentative Schedule:

March 25 (Thursday): Sendai Excel Hotel Tokyu

15:30 -	Registration
16:00 - 16:10	Opening session
16:10 - 17:40	Evening plenary session
18:00 - 20:00	Dinner/Mixer

March 26 (Friday): Sendai International Center

09:00 - 10:30	Morning plenary session
10:50 - 12:20	Parallel sessions
12:20 - 15:30	Poster session and Discussion
15:30 - 17:45	Afternoon special session

March 27 (Saturday): Sendai International Center

09:00 - 10:30	Morning plenary session
11:00 - 12:30	Parallel sessions
13:30 - 15:00	Parallel sessions
15:30 - 17:00	Afternoon plenary session
17:00 - 17:15	Closing remarks
18:00 - 20:00	**Banquet: Sendai Excel Hotel Tokyu**

Tentative list of Invited speakers:

Pulikel M. Ajayan, Rice University, USA
Masayoshi Esashi, WPI-AIMR
Hans-Joerg Fecht, Ulm University, Germany
Alan Lindsay Greer, University of Cambridge, UK
Chikara Hayashi, ULVAC, Inc.
Zhaomin Hou, RIKEN Advanced Science Institute
Akihisa Inoue, Tohoku University
Do Hyang Kim, Yonsei University, Korea
Brian Korgel, University of Texas, USA
Jörg F. Löffler, ETH, Switzerland
Thaddeus B. Massalski, Carnegie Mellon University, USA
Gerhard Meyer, IBM Zurich, Switzerland
Yoshio Nishi, Stanford University, USA
Matthew J. Rosseinsky, University of Liverpool, UK
Jan Schroers, Yale University, USA
Masatsugu Shimomura, WPI-AIMR
H. Eugene Stanley, Boston University , USA
Zhigang Suo, Harvard University, USA
Takashi Takahashi, WPI-AIMR
Hajime Tanaka, The University of Tokyo
Richard Tilley, Richard Tilley, New Zealand
Yasuteru Urano, University of Tokyo
James J. Watkins, University of Massachusetts, USA
Alain Reza Yavari, Institute National Polytecnique de Grenoble, France
Jing Zhu, Tsinghua University, China

Junior Faculty/Post-doctoral Positions

Tohoku University
WPI-AIMR

Effective October 1, 2007, Tohoku University created a new Research Institute, the Advanced Institute for Materials Research (AIMR), based on an initiative of the Japanese Department of Education (MEXT) for World Premier International Research Center Initiative (WPI) to bring together scientists involved in research on nano-science and technology.
In the 21st century, material science, broadly defined as the study of how complex/novel properties arise in matters/materials from the interactions of individual components, will comprise of inter-discipline collaboration.
(HTTP://WWW.WPI-AIMR.TOHOKU.AC.JP).
Over the next few years, as many as one hundred new appointments at the levels of post-doctoral fellows and junior faculty will be available. All innovative researchers are welcome as active promoters of basic/applied sciences in the fields of physical metallurgy, physics, chemistry, precision mechanical engineering and electronic / informational engineering.

We are continuously looking for excellent applicants throughout the year.
Please submit

1) **a curriculum vitae,**
2) **research proposal (<3,000 words),**
3) **summary of previous research accomplishments (<2,000 words),**
4) **copies of 5 significant publications, and**
5) **2 letters of recommendation**

by email to
wpi-office@bureau.tohoku.ac.jp
（Chemists） **yoshi@mail.tains.tohoku.ac.jp**
（Physicists） **sakurai@imr.tohoku.ac.jp.**
All files must be submitted electronically in pdf or Word format.

Applications from, or nominations of, women and minority candidates are encouraged. Tohoku University WPI-AIMR is an affirmative action / equal opportunity employer.

Graduate Student scholarship
In Materials Science/Engineering

WPI-AIMR
Graduate Student scholarship

Effective October 1, 2007, Tohoku University created a new Research Institute, the Advanced Institute for Materials Research (AIMR), based on an initiative of the Japanese Department of Education (MEXT) for World Premier International Research Center Initiative (WPI) to bring together scientists involved in research on nano-science and technology.

In the 21st century, material science, broadly defined as the study of how complex/novel properties arise in matters/materials from the interactions of individual components, will becomes an essential and most important research topics

(HTTP://WWW.WPI-AIMR.TOHOKU.AC.JP).

TU WPI-AIMR is now looking for young motivated Ph.D. graduate student candidates in the fields of physical metallurgy, physics, chemistry, mechanical engineering and electronic / informational technology. All innovative M. S. students are welcome as active promoters of basic/applied sciences in these fields.

Applications are continuously screened throughout the year.
Please submit

1) **a curriculum vitae,**
2) **research proposal (<1,000 words),**
3) **2 letters of recommendation,**

by email to
wpi-office@bureau.tohoku.ac.jp
（Chemists） **yoshi@mail.tains.tohoku.ac.jp**
（Physicists） **sakurai@imr.tohoku.ac.jp.**
All files must be submitted electronically in pdf or Word format.

WPI-AIMR

Workshop Guideline

Tohoku University's new Research Institute, the Advanced Institute for Materials Research (WPI-AIMR) solicits several applications per year for International Workshops in the field of "broadly defined Materials Science."

Guidelines:

1) Organizers

Qualified research staff of academic institutions and public or private research establishments can submit the application for an international workshop to be held at WPI-AIMR or its Satellite branches, jointly with the WPI-AIMR principal investigator(s) whose research interest overlaps with the scope of the workshop.

2) Financial support

Under normal circumstances, WPI-IMR supports up to 2/3 of the workshop budget, while the organizer is expected to cover the rest.

3) deadline

The application must be received at least four months in advance

to

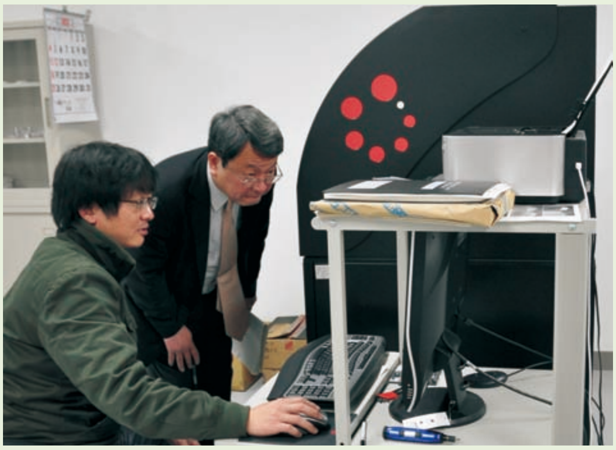
wpi-office@bureau.tohoku.ac.jp
（Chemists） **yoshi@mail.tains.tohoku.ac.jp**
（Physicists） **sakurai@imr.tohoku.ac.jp**.

All files must be submitted electronically in pdf or Word format.

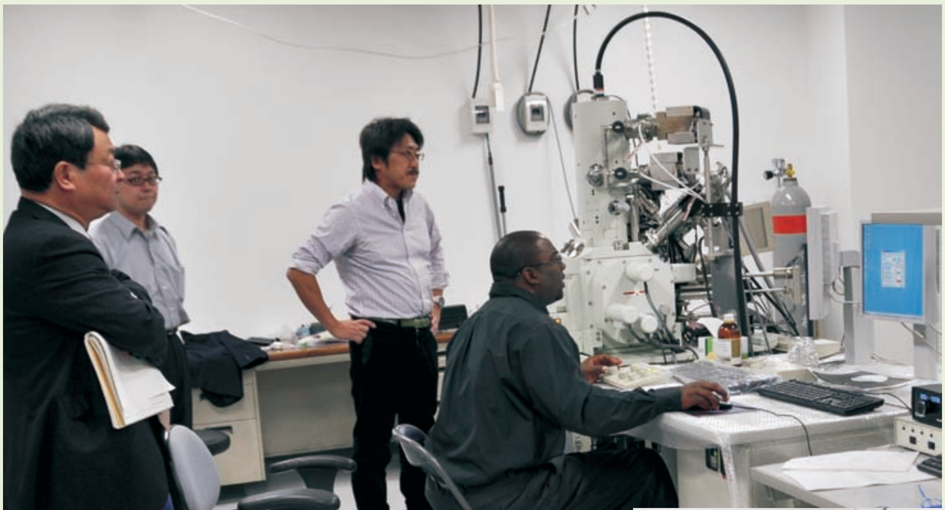
Appendix

Chen Group (BMG)

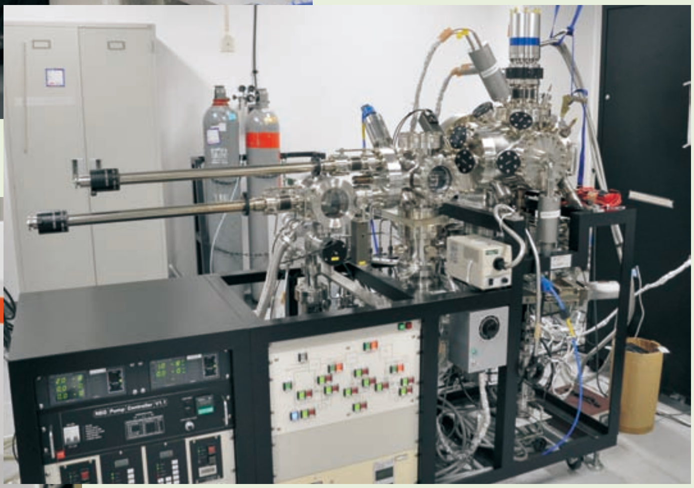
Transmission Electron Microscope (TEM)



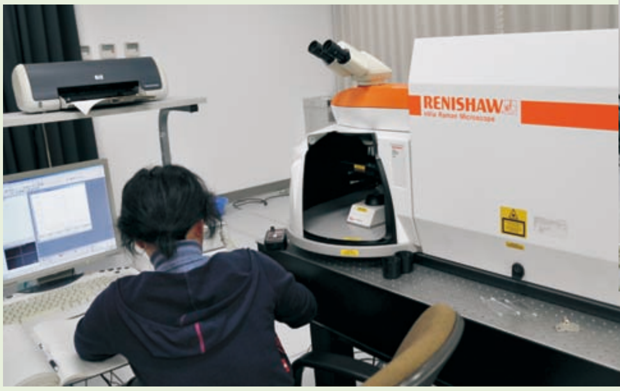
TMS G200 Nanoindentation System



Dual beam SEM-FIB system



Atom Probe



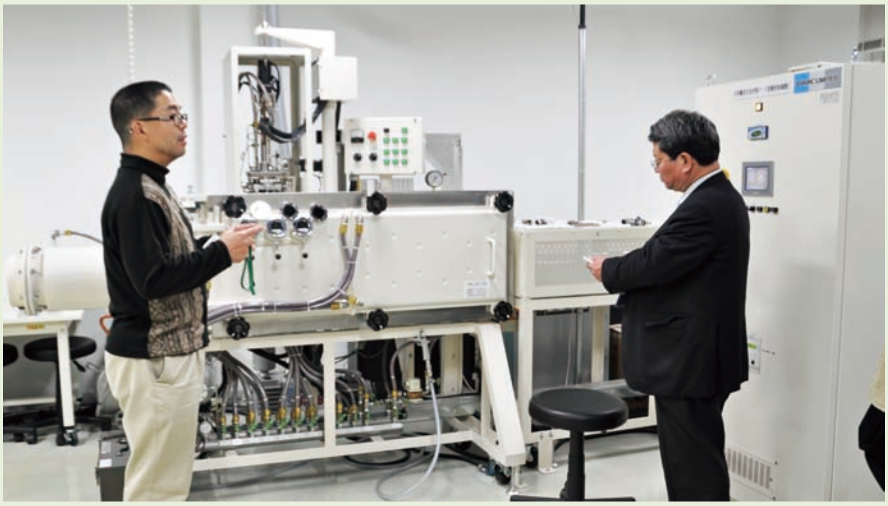
Raman Spectroscopy System

Group Photo

Louzguine Group (BMG)

A Single-Mode Applicator for Microwave Processing of Materials under Pressure in a Controlled Atmosphere

BMG Exhibition Room



Mass Production Machine for Master Alloy Fabrication

(Patent Pending: It has been developed jointly by YKK Corporation and Tohoku University)

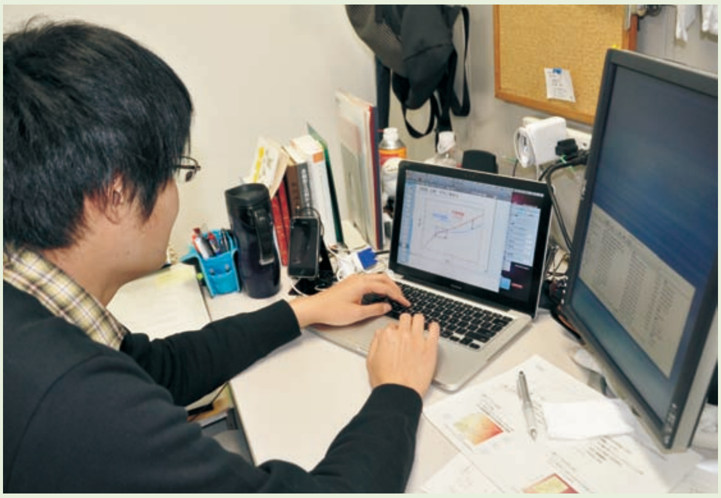
Cleanbooth for BMG Application Products

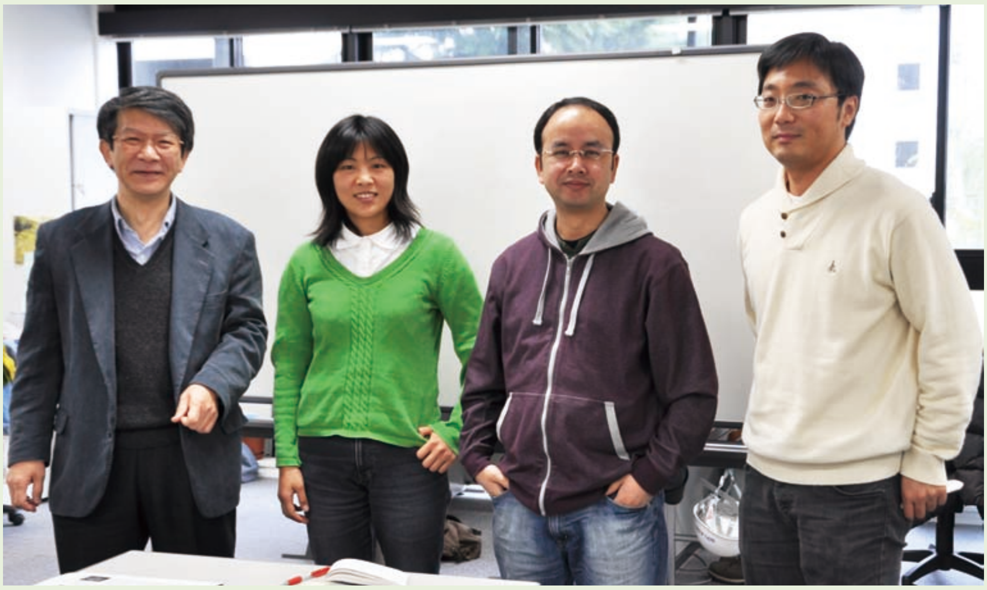
Differential Scanning Calorimeter
(Perkin Elmer DSC8500)

Group Photo (Dr. Madge, third from left, from Greer Group)

Tokuyama Group (BMG)

Laboratory Meeting



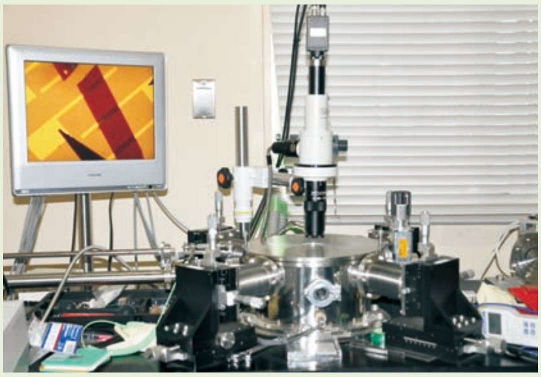


Group Photo

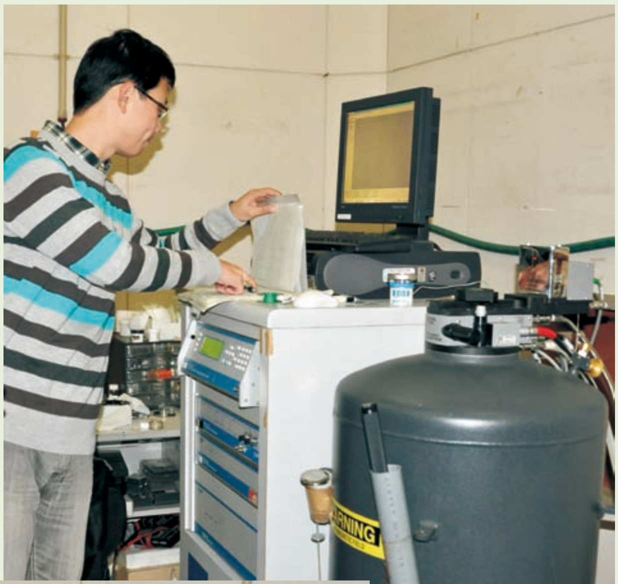
Tanigaki Group (Nanophysics)

Glove Box

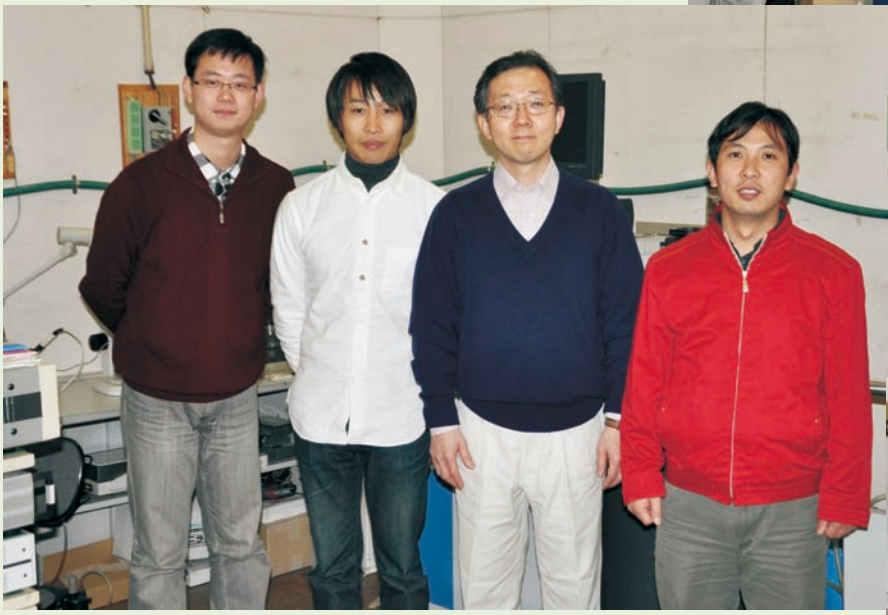
Wire Bonder



Cryogenic probe system



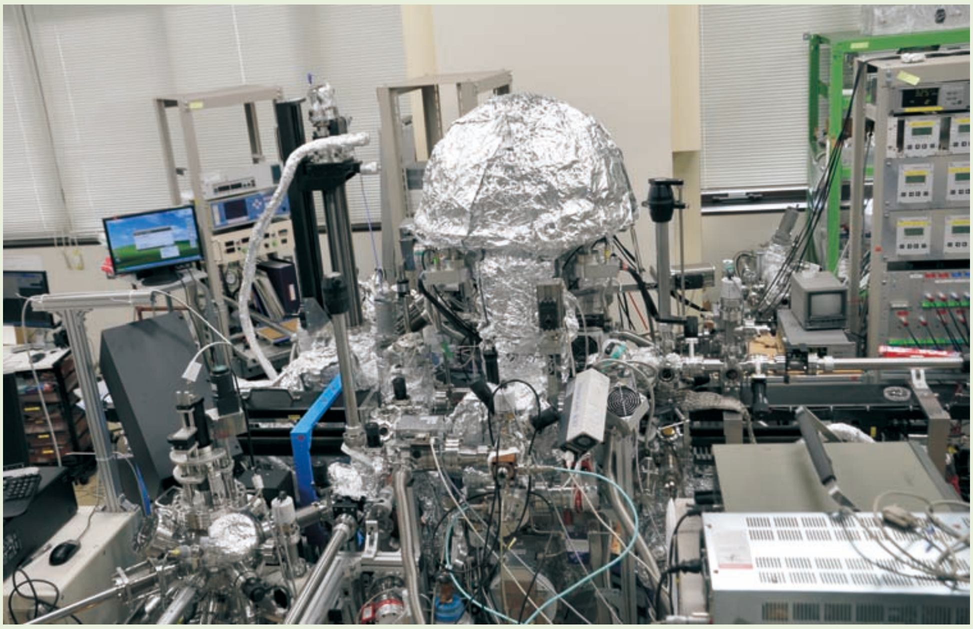
Physical Property Measurement System (PPMS)



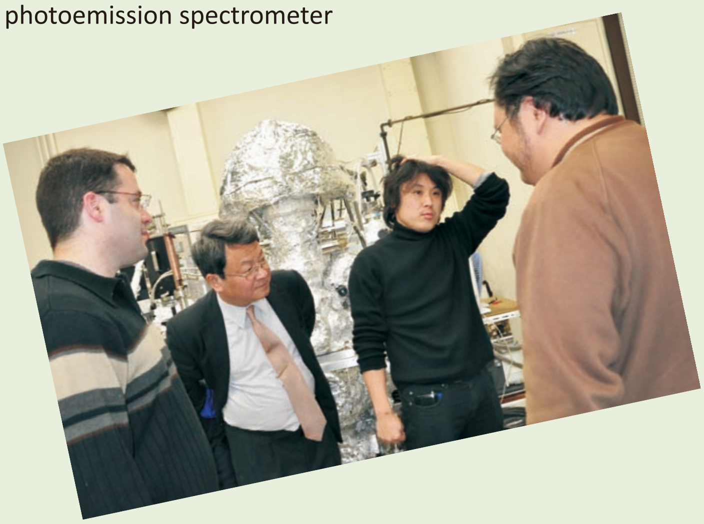
Group Photo

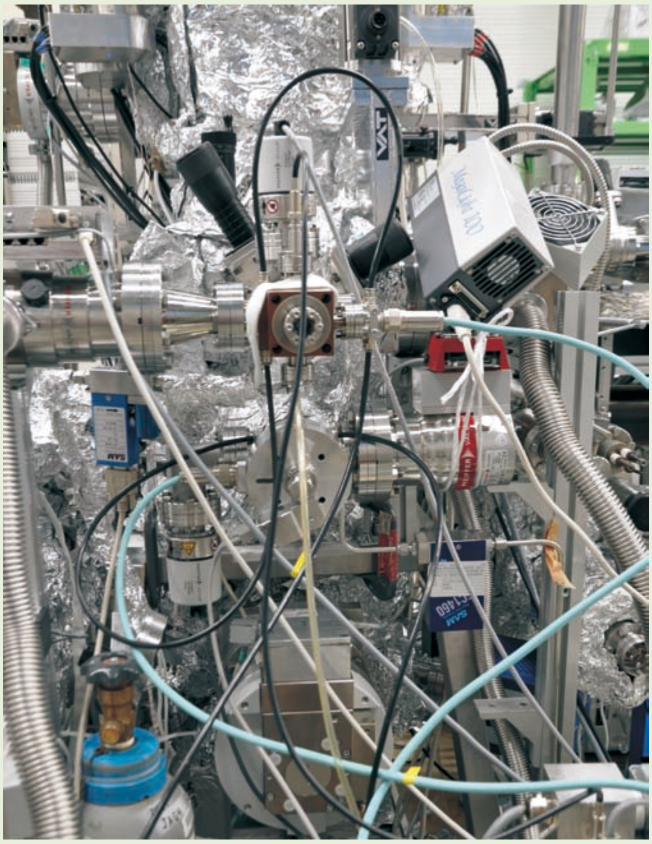
Magnetic Property Measurement System (MPMS)

Takahashi Group (Nanophysics)

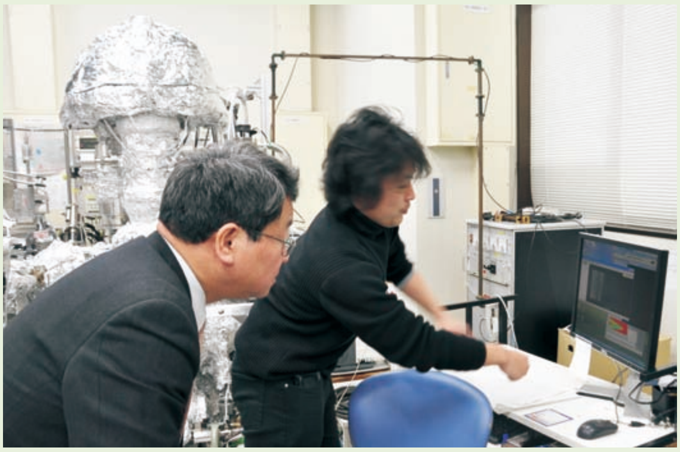


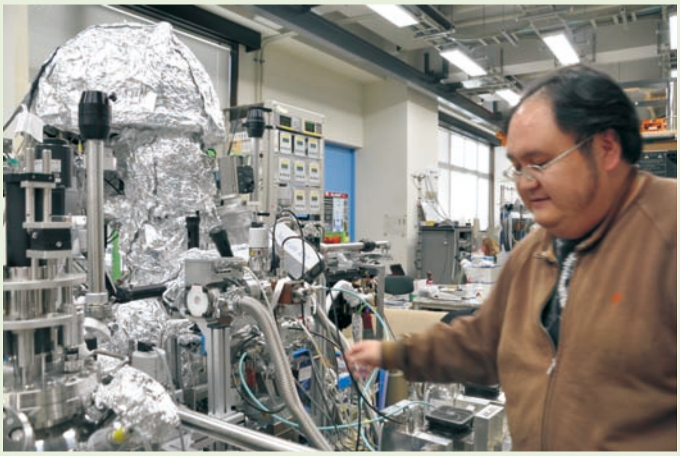
Spin-resolved high-resolution photoemission spectrometer

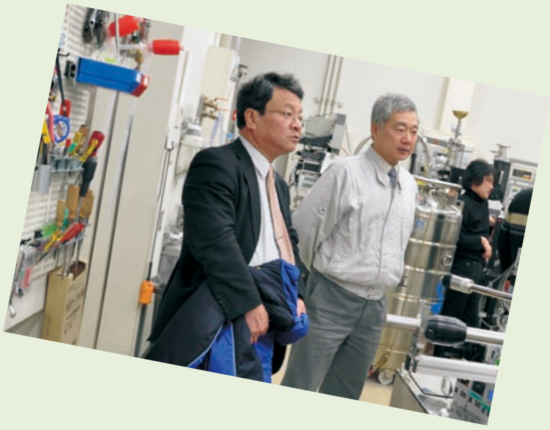


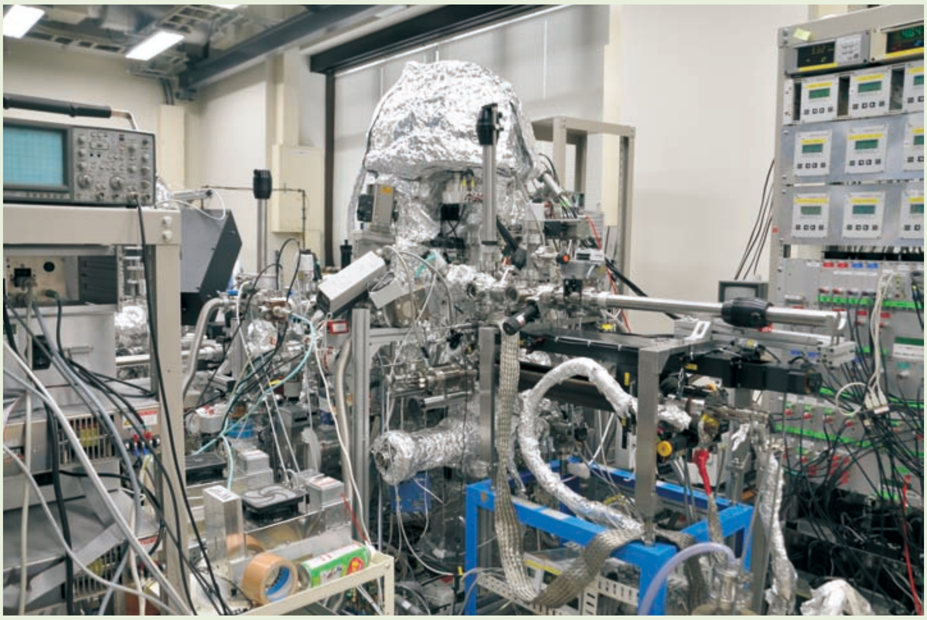


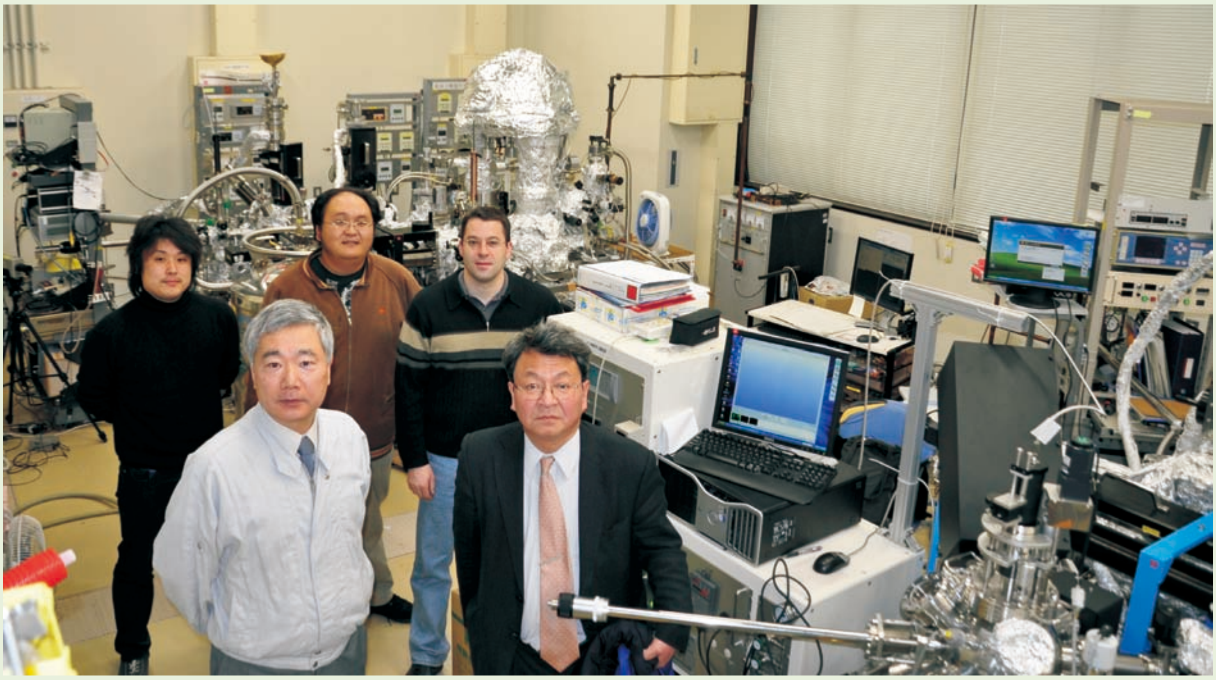
High-intensity xenon plasma discharge lamp







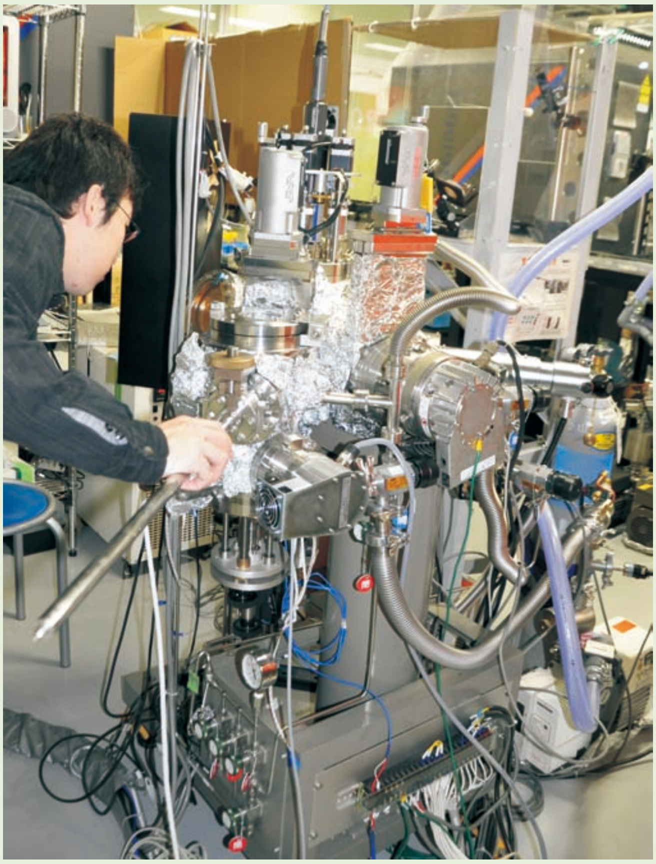




Group Photo

Kawasaki Group (Nanophysics)

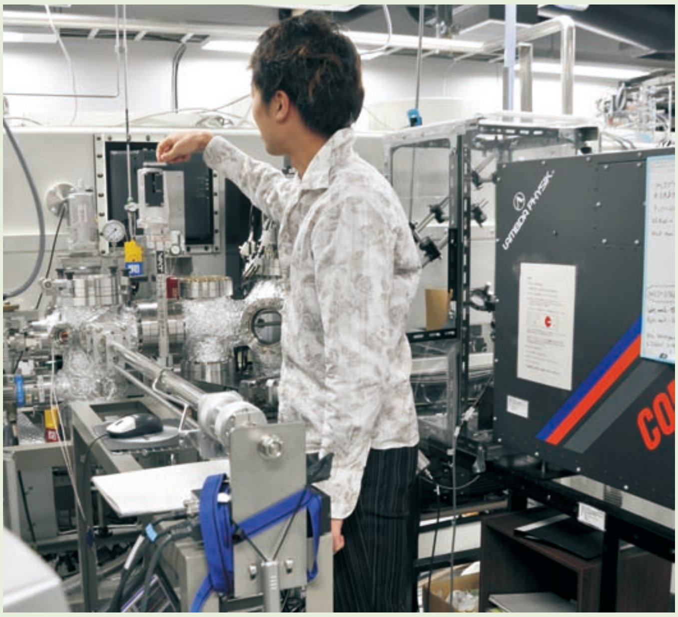
Scanning Electron Microscope (SEM)



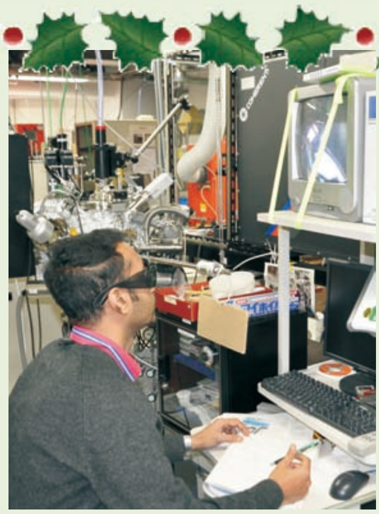
Laser Molecular Beam Epitaxy System

Semiconductor Prober & Analyzer System

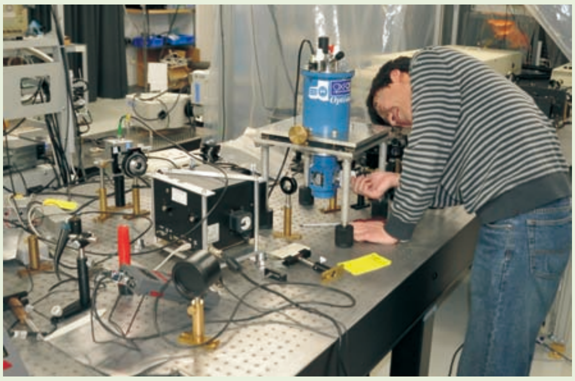
Atomic Force Microscope (AFM)



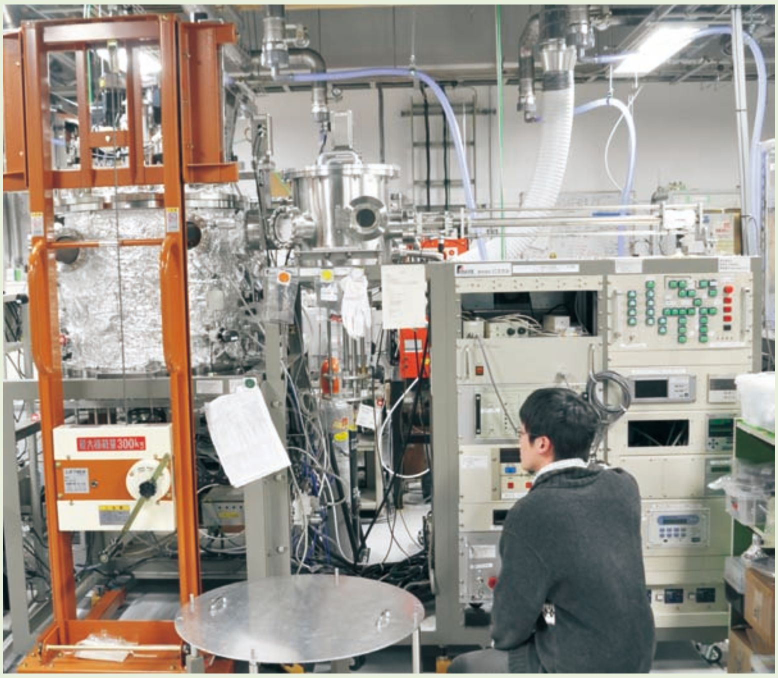
Laser Molecular Beam Epitaxy System



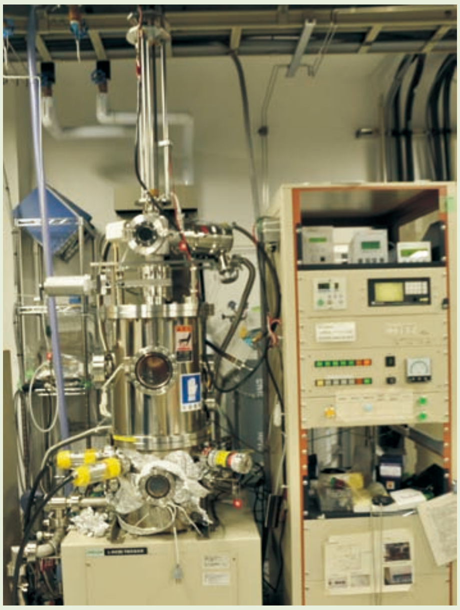
Laser Molecular Beam Epitaxy System (SEM)



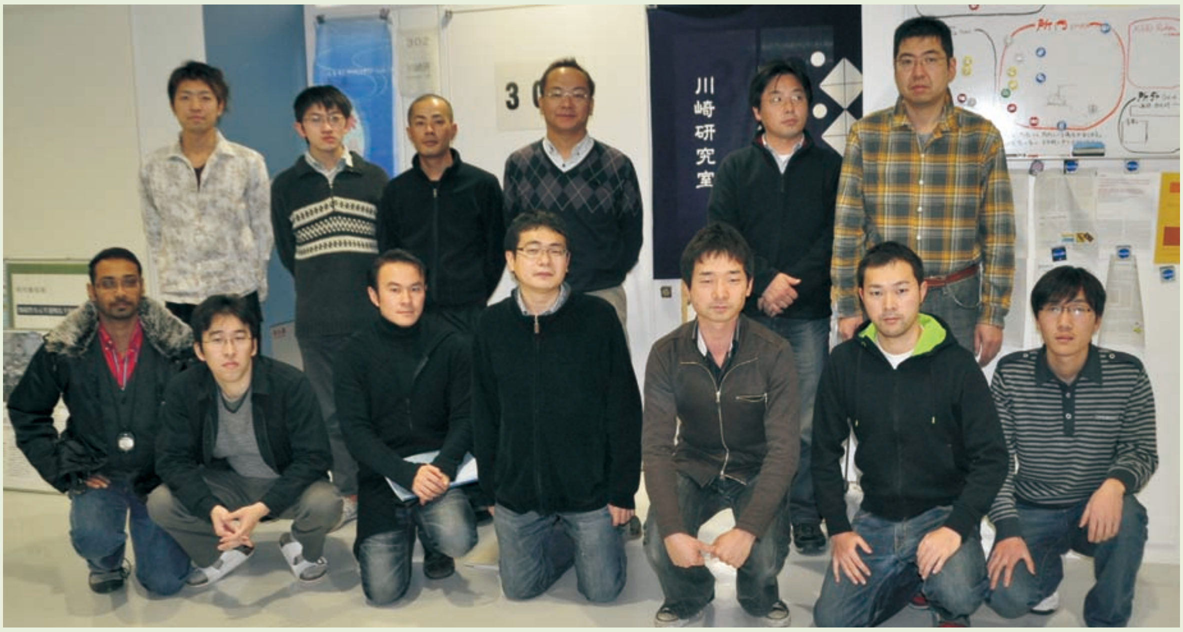
Cryogenic Optical Measurement System



Combinatorial Sputter System

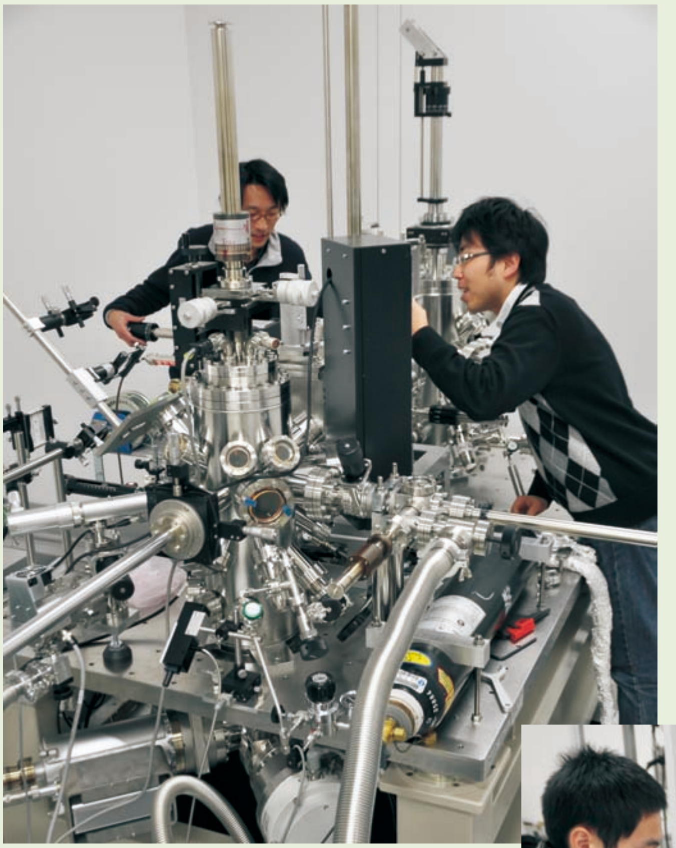


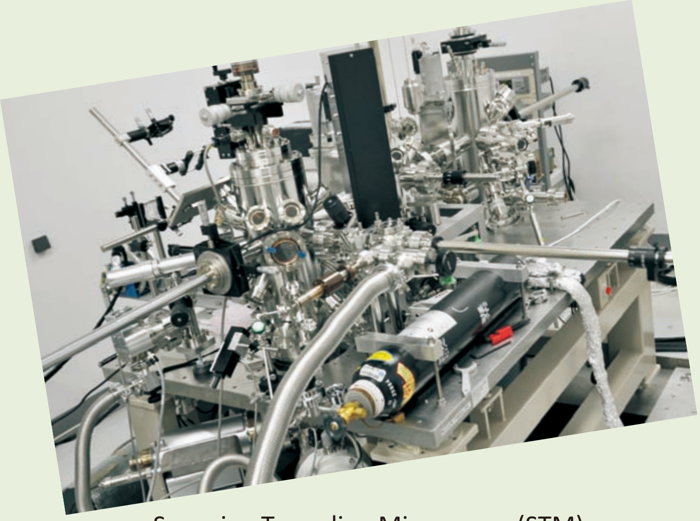
EB evaporator



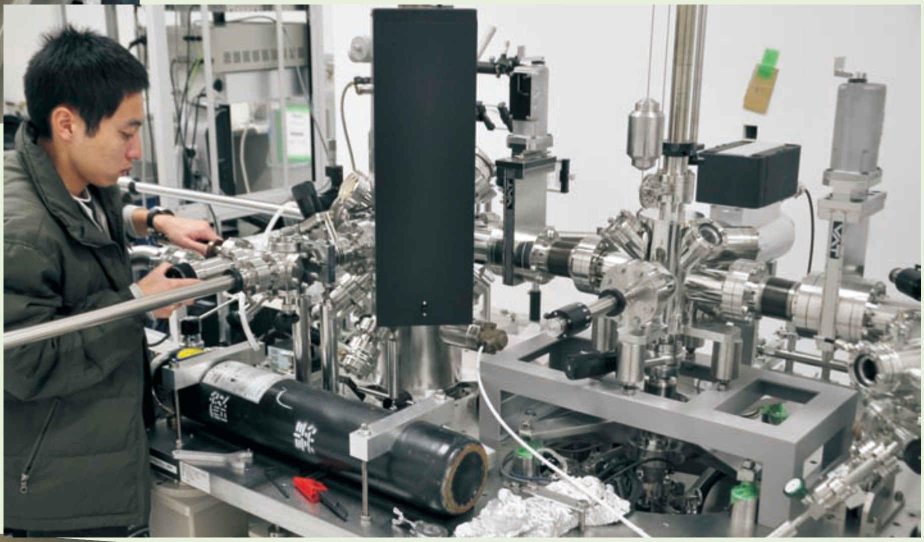
Group Photo

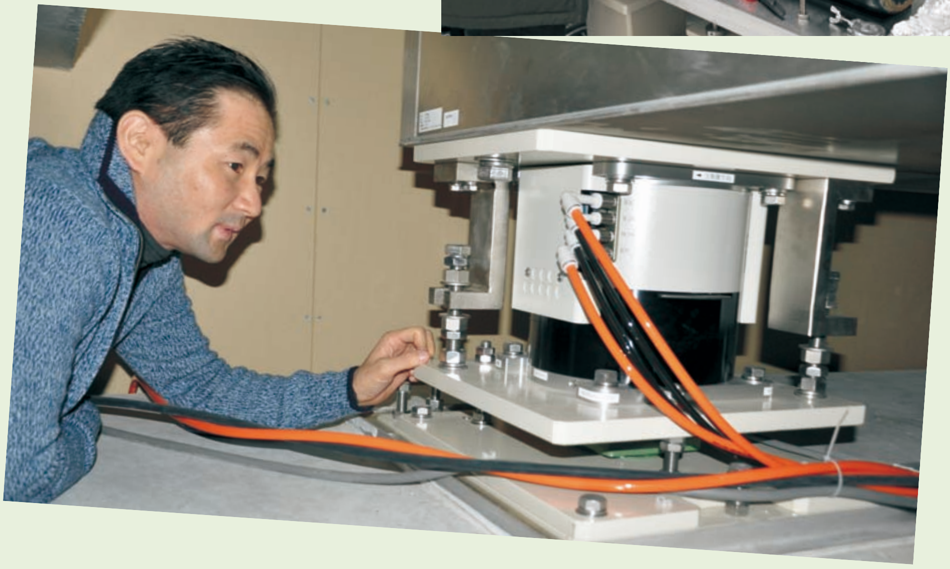
Hashizume Group (Nanophysics)

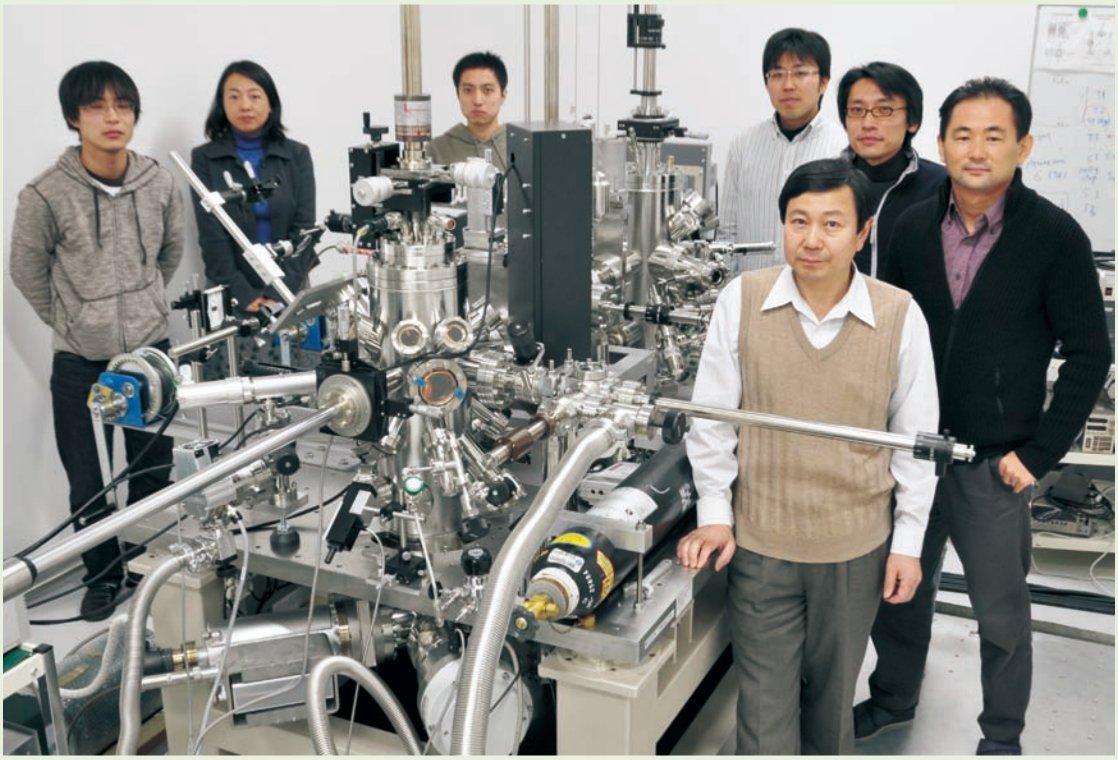




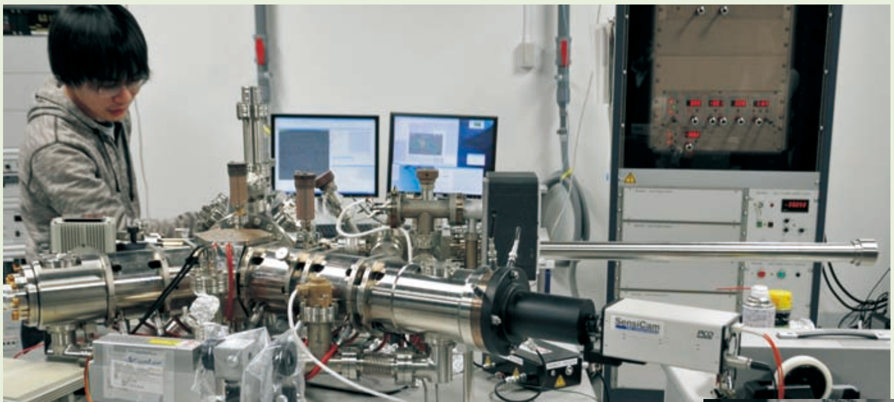
Scanning Tunneling Microscope (STM)



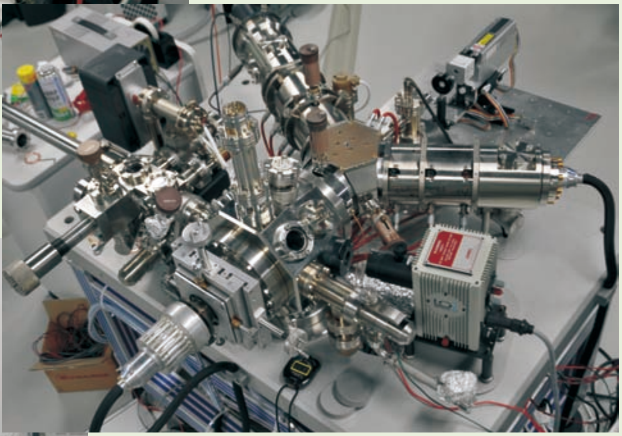


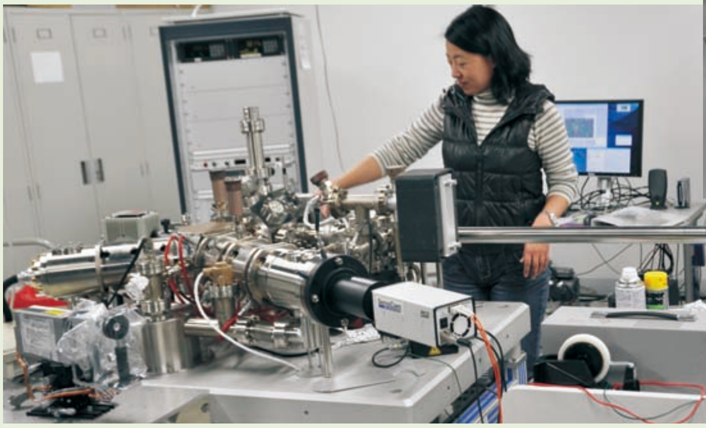


Group Photo (Dr. Liu, second from left, from Xue Group)



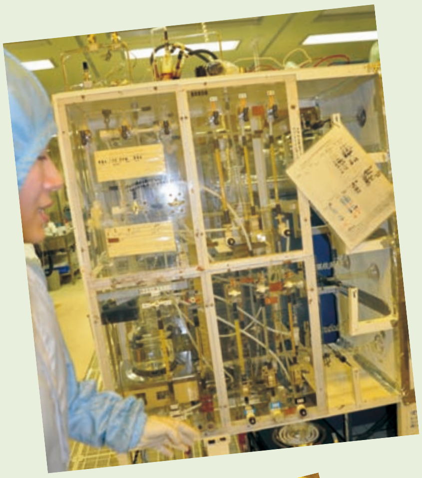
Low Energy Electron Microscope (LEEM)





Esashi Group (Device/ System)

Homemade oxidation furnace



PZT Metal Organic Chemical Vapor Deposition (MOCVD)

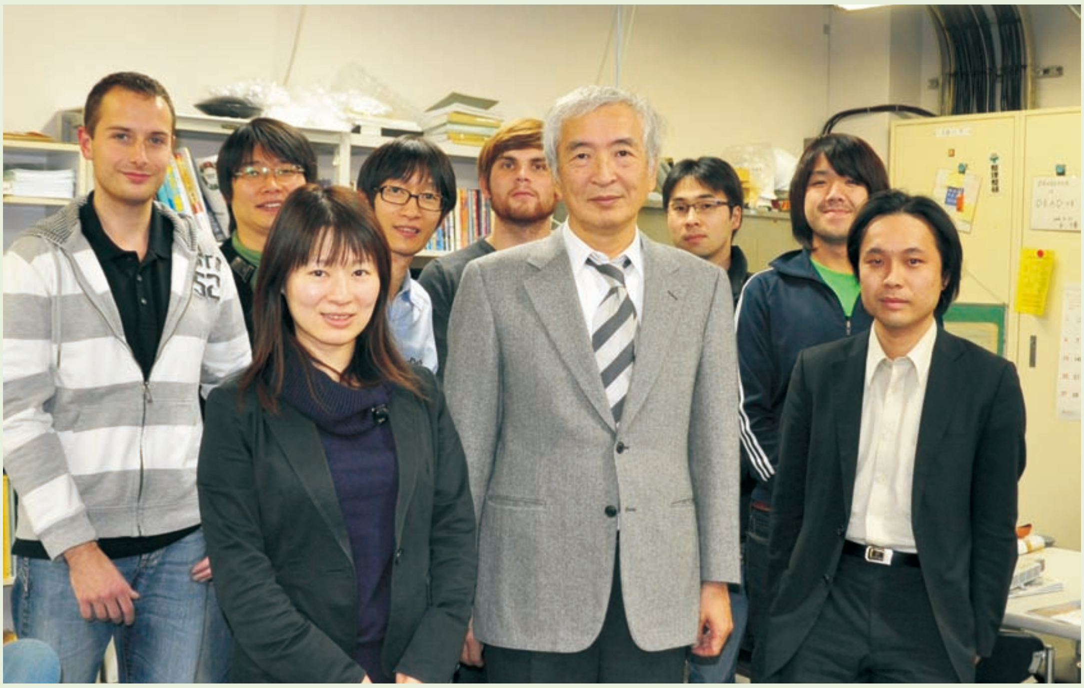
Chemical hood

Hot-Filament CVD

Research staff of Esashi Group

Homemade sputtering equipment

Research staff from Gessner Group



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2009 WPI-AIMR News

Contents

(Volume - page)

Interviews

Honorary Degree Ceremony for Prof. V. Narayanamurti on May 22, 2009

News Update

Open House Ceremony of Integration Laboratory on May 22, 2009

The New WPI Joint Seminar Series by M. Tsukada & T. Hashizume

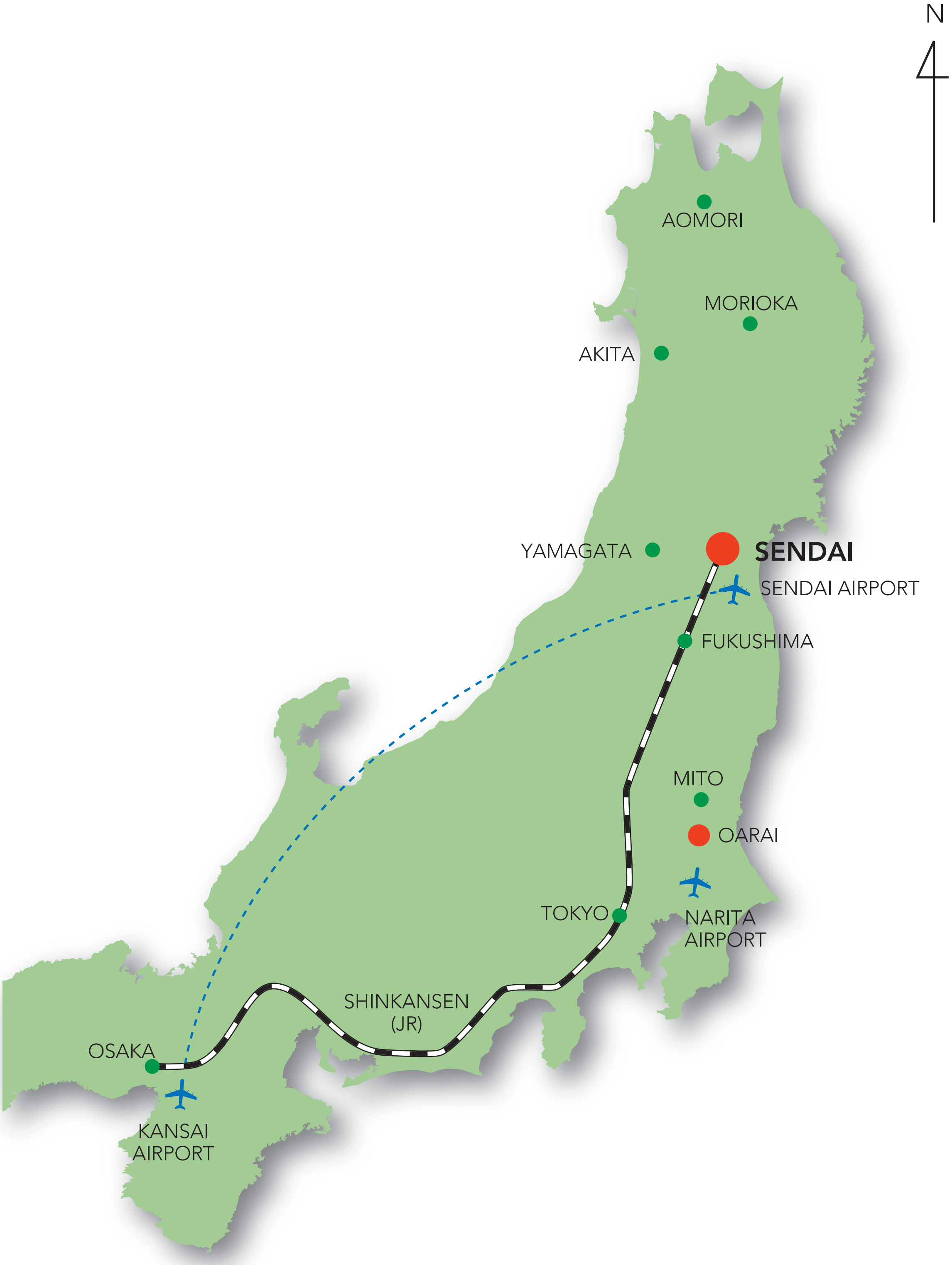
(Seminar Summary)

Research Prospect

WPI-IFCAM

Announcement

Appendix



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