WPI-AIMR / Cambridge Workshops and Discussions on "Hierarchical materials for green energy"

Wednesday 20 November 2013-11-13

09:30	Plenary session in the Jan Evetts Meeting Room.
	Prof. Kotani — Welcome
	Prof. Greer — Introduction to the Dept of Materials Science & Metallurgy
10:00	Separate Discussion Groups (see the reports attached)
12:00	Break and report writing
12:30	Tour of DMSM new building
13:00	Lunch
13:45	Plenary Session in Goldsmiths Room 2
	Dr Krzystof Koziol On carbon nanotubes to replace copper as conductors
	Dr Sohini Kar-Narayan On energy harvesting
	Dr Stoyan Smoukov On active and intelligent materials
14:45	End of visit to Dept. of Materials Science & Metallurgy
15:00	Arrival at the Department of Chemistry on Lensfield Road
15:15	Presentation by Dr Demeter Kiss
	(Dept of Pure Mathematics and Mathematical Statistics)
15:30	Presentation by Prof. David Wales (Dept of Chemistry)
16:00	Closing discussions

Report of Discussion Meetings at AIMR/Cambridge Workshop

November 20, 2013
At Department of Materials Science and Metallurgy
and Department of Chemistry, Cambridge University

Attendee from AIMR: M. KOTANI, M. TSUKADA, N. ASAO, A. HIRATA T. HITOSUGI,
S. MIZUKAMI, S. SOUMA, K. AKAGI, Z. WANG, N. AOKI, R. JOKSIMOVIC, Y. NAKAMICHI

Group 1: *Materials Modelling*
Cambridge: Dr Paul Bristowe, Dr James Elliott
AIMR: Dr Akagi, Prof. Kotani, Dr Wang, Prof. Tsukada, and others

Group 2: *Functional Materials*
Cambridge: Prof. J. Driscoll, Prof. N. Mathur, Dr Z. Barber, Dr X. Moya,
Dr S. Kar-Narayan and the Device Materials Group
AIMR: Dr T. Hitosugi, Dr S. Mizukami, and others

Group 3: *Electron Microscopy*
Cambridge: Prof. P. Midgley, Dr C. Ducati, Dr R. Langford (Dept. of Physics)
AIMR: Prof. A. Hirata, and others

Group 4: *Topological Insulators*
Cambridge : Dr M. Saxena and his group, AIMR: Dr S. Souma, and others

Group 5: *Chemistry*
Cambridge: Dr K. Orchard, Dr J. Zhang, Dr S. Smoukov
AIMR: Prof. N. Asao, and others

Report of Discussion Meeting –Group 1-

Participants at the meeting: Dr. Bristowe, Dr. Elliott and Akagi, Wang, Tsukada, Kotani

Research Topics discussed (short title): material modeling based on computation

Keywords of materials, methods, phenomena and others:
first-principles calculation, multi-scale modeling

Dr. Bristowe is a specialist of the first-principles calculations with advanced approaches such as exact-exchange methods, self-interaction correction and so on. He gave five topics from his recent studies. Accurate description of electronic structure of Co-based perovskite materials for SOFC (Solid-Oxide Fuel Cell) electrodes, analysis on mechanical property of Ni-based superalloys for the aircraft industry and exploration of metal-organic framework structures for "gas storage / gas separation" are examples of them. The last one (metal-organic framework structure) is attractive to me(Akagi), because it could be one of the possible applications to the gas separator which is a key component for Li-air batteries I am studying with Chen-group. He showed interest in my research topics on Rh doped $SrTiO_3$ materials for photolysis of water and structure analysis of Co doped TiO_2 systems.

Dr. Elliott is a math-mate researcher. He is a specialist of multi-scale computer modeling and showed a wide variety of topics such as aggregation of calcite in water, formation of biomineral nano-structure, confinement effect on collagen-based materials and powder compaction for medicine tablet. The former two topics are aqueous systems, in which my study on interaction between ionic species and a hydrogen-bond network of water. He also expressed a strong interest in my recent result which elucidates a certain type of hydrogen-bond structures play a role of effective repulsive potential for hydrogen ions. Report by Dr. K.Akagi

Report of Discussion Meeting -Group 2-

Participants at the meeting: T. Hitosugi, and S. Mizukami, Prof. J. L. MacManus-Driscoll, and a member from Prof. Blamire group

Research Topics discussed (short title): Discussed on oxide and spintronics

Keywords of materials, methods, phenomena and others: oxide, spintronics

Brief Summary of Discussions: Prof. MacManus-Driscoll introduced us that the strained epitaxial BiMnFeO3 films grown by PLD have very high ferromagnetic transition temperature over 600K, which is very promising to apply the spin-filter devices based on magnetic tunnel junctions. We discussed the possibility to make the devices, such as Fe/MgO/BiMnFeO3/magnetic-electrode. Moreover, her post doctor introduced his planar devices using magnetic multilayer with superconducting electrode, which enable him to investigate superconducting current controlled by magnetization alignment, i.e., anti-parallel and parallel magnetizations for two ferromagnetic layers. This project is still in progress. It is so interesting concept, so that we considered the chance of collaboration. Further, we visited atomic layer deposition system which operates in ambient air. The system have capability to deposit TiO2 and other materials in atomic layer precision. They can introduce Nb dopant into TiO2 to make transparent conductors.The system seems good for making large size films with less inhomogeneity. What was surprising was that the effect of contamination is negligible for their purpose. Report by Dr. Hitosugi

Report of Discussion Meeting –Group 3-

Participants at the meeting: Prof. P. A. Midgley, Dr. C. Ducati, Dr. R. Langford (Cambridge), Dr. A. Hirata (AIMR)

Research Topics discussed: Installation environment of advanced electron microscopes

Keywords of materials, methods, phenomena and others: Electron microscopy

Brief Summary of Discussions:

The new facilities of transmission electron microscopes (TEM) in Cambridge were introduced by Prof. Midgley and Dr. Ducati. The state-of-the-art TEM (FEI Titan) with Cs-corrector and monochrometer has been installed in the special room. Moreover there are several similar rooms which are made large enough to accommodate any advanced TEM. We discussed installation environment of advanced TEMs, e.g. basement, antiseismic system, noise reduction system, and magnetic canceller system. It is striking that the basement, which is separated from the main building, is the second largest concrete block in UK. We also discussed some new data about oxide interface and metallic Laves phase obtained by Titan.

Report by Dr. Hirata

Figure: New room for advanced TEM (left) and newly-installed FEI Titan Cs-corrected TEM (right).

Report of Discussion Meeting -Group 4-

Participants at the meeting: S. Souma (WPI), Prof. Saxena Montu, his student (Cambridge)

Research Topics discussed (short title): Quantum criticality, Topological superconductivity

Keywords of materials, methods, phenomena and others:

Quantum criticality (STO, $SrRu_2O_4$), Fermiology, and Topological superconductor (material in secret)

Brief Summary of Discussions:

1. Quantum criticality (QC): Applying high-pressure for tuning band-gap of semiconductor at Cambridge, which is crucial to observe QC phenomena. ARPES with applying pressure (developing at Tohoku) would contrite such control of electronic band.

2. Fermiology of various materials: Sazena group is one of top experimentalist for research of Fermi surface using self-developed low-temperature dHvA instruments; $SrRu_2O_4$, $SrVO_3$, UPt_3, MgB_2,…; some of those are p-wave superconductor, candidate of topological superconductor.

3. We discuss how to observe the majorana surface state of topological superconductor. Saxena group is now developing candidate material. We will keep in touch for future collaboration work about electronic structure of topological superconductor.

Report by Dr.Souma

Report of Discussion Meeting -Group 5-

Participants at the meeting: N. Asao, N. Aoki, K. Orchard, J. Zhang, R. Joksimovic

Research Topics discussed (short title): water oxydation by photocatalysis / nanotribology and redispersion of nanoparticles

Keywords: photocatalysis, surface forces, nanotribology, supercrititical synthesis

Brief Summary of Discussions:

- The current research topic carried out at Cambridge Joint Laboratory on the water oxidation by photocatalysis was discussed. Relevant suggestions for improvement in dye molecule design and study, and electrode preparation were made.

- Discussion involving the use of biocatalysts (Photosystem II) for water oxidation in fundamental photoelectrochemical characterisation studies. In particular, strategies involving enzyme immobilisation were discussed to improve the immobilisation on electrodes.

- Discussion on the cooperation between the Kurihara lab and the Adshiri lab:
Cubic ceria nanoparticles coated with decanoic acid are being synthesized by the Adshiri group under supercritical conditions. In the Kurihara group, we perform surface forces measurements by the SFA (surface force apparatus) and also resonance shear measurements to investigate the nanotribological properties of the nanoparticles. Resonance shear results point towards good lubricant properties of the particles.

- We also discussed the relation between flow, fluid, and nanoparticle formation and nanofluid physical properties. Mixing of reactants is significant to control the particle size as well as the selectivity of organic synthesis. Nanoparticle aggregation is one problem faced in the context of this research. For this reason, it is important to design an effective redispersion process. The measurement method of the viscosity of the nanofluid was also discussed. The relationship between bulk and microscopic physical properties is relevant, and this aspect needs modeling of such systems to establish a science of nanofluid. Report by Prof. Asao