SYCO 1: Mechanically controlled electrical conductivity of oxides

Time: Monday 9:30–12:30 Location: H1

Invited Talk SYCO 1.1 Mon 9:30 H1

Dislocation Dynamics and Their Conductivities in Oxides — •Yuichi Ikuhara — Institute of Engineering Innovation, The University of Tokyo, Tokyo, 113-8656, Japan — Nanostructures Res. Lab., Japan Fine Ceramics Center, Nagoya, 456-8587, Japan — WPI-AIMR Research Center, Tohoku University, Sendai, 980-8577, Japan

Dislocations can be used as conductive nanowires in crystals [1]. In this study, insulating sapphire and YSZ ($Y_2O_3 - ZrO_2$) single crystal are used as model systems in which high-density of dislocations and periodically aligned dislocations were introduced by high-temperature compression tests and fabrication of bicrystals with low-angle grain boundaries. The electron and ion conductivities were measured for the dislocation introduced crystals, and it was concluded that the techniques are very useful for providing new functions such as electron and ion conductivities. We call these techniques as *Dislocation Technology*. It is also interesting to directly observe the dislocation motion. In this study, the nanoindentation experiments were conducted for $SrTiO_3$ bicrystals inside TEM (Transmission Electron Microscope). The bicrystals including various types of GBs were prepared for the experiments. The samples were indented with the sharp diamond tip and successfully observed the dislocation dynamics [2]. It was found that the interaction between the introduced lattice dislocations and the GBs were dependent on the GB characters.

[1] Y.Ikuhara, Prog. Mater. Sci., 54, 770 (2009)

[2] S. Kondo, T. Mitsuma, N. Shibata, Y. Ikuhara, Sci. Adv., 2(11), 1501926 (2016).

Invited Talk SYCO 1.2 Mon 10:00 H1

Strain effects in ionic conductivity and electrode processes — •Jürgen Janek[1] and Carsten Korte[2] — [1]Institute of Physical Chemistry, Justus-Liebig University, Gießen, Germany — [2]Institut für Energie- und Klimaforschung (IEK), FZ Jülich, Germany

Strain induced effects play an important role in solid state reactions and transport processes. Strain may be caused by external mechanical load or by chemical reactions in the solid state itself. In this presentation two examples for strain effects in the solid state will be highlighted: a) Strain created during growth of hetero-multilayers of ion-conducting solid electrolytes can cause conductivity changes relative to the unstrained bulk, but due to the complex microstructure of heterophase multilayers it is difficult to separate strain effects from the effect of dislocations, grain boundaries and interfaces [1]. b) Strain created by volume changes of intercalation compounds in composite cathodes of solid state batteries (chemo-mechanics) causes severe interface impedances that deteriorate the performance of solid state batteries [2].

[1] J. Keppner et al., Phys. Chem. Chem. Phys. 20 (2018) 9269

[2] R. Koerver, et el., Ener. Environ. Sci. 11 (2018) 2142

Invited Talk SYCO 1.3 Mon 10:30 H1

Elastic dipoles of point defects in materials — •Celine Varvenne[1], Thomas Jourdan[2], and Emmanuel Clouet[2] — [1]CINaM - Aix Marseille Univ./CNRS, Marseille, France — [2]SRMP - CEA Saclay, Gif-sur-Yvette, France

Point defects in crystalline solids, such as vacancies, self-interstitials, solute atoms or small clusters, play a central role in controlling materials properties and their kinetic evolutions. The knowledge of the elastic dipole of a point defect, a second rank tensor fully characterizing the point-defect, allows one to directly obtain the long-range elastic field induced by the point-defect and its interaction with other elastic fields. Here, we will detail how to properly parameterize such an elastic model - either from experiments or from atomistic simulations [1] - which is an important first step for subsequent quantitative modeling. We will address both neutral defects in metals and alloys, and charged defects in semiconductors or insulators. Several applications will then be presented, focusing on finite-size corrections schemes in ab initio calculations, elastodiffusion effects and bias calculations [2,3].

[1] E. Clouet et al., Acta Mater. 56 (2008); Nazarov et al. Phys. Rev. B 94 (2016); C. Varvenne & E. Clouet, Phy. Rev. B 96 (2017)

[2] C. Varvenne, F. Bruneval, M.-C. Marinica, E. Clouet, PRB 86 (2013); F. Bruneval, C. Varvenne, E. Clouet, J.-P. Crocombette, Phys. Rev. B 91 (2015)

[3] A. Vattré et al., Nat. Comms. 7 (2016); E. Clouet, C. Varvenne & T. Jourdan, Comp. Mat. Sci. 147 (2018)

Coffee break

Invited Talk SYCO 1.4 Mon 11:30 H1

Mapping strain/pressure with ZnO nanowire arrays by piezo-phototronic effect — •Caofeng Pan — Beijing Institute of Nanoenergy and Nanosystems,Chinese Academy of Science

Emulation of human senses via electronic means has long been a grand challenge in research of artificial intelligence as well as prosthetics, and is of pivotal importance for developing intelligently accessible and natural interfaces between human/environment and machine. In this talk, we present a novel design of ZnO nanowire arrays, which can be used to directly record the strain distribution by piezotronic and piezo-phototronic effect. First, we demonstrated how the piezo-phototronic effect can be effectively utilized to enhance the emission intensity of an n-ZnO/p-GaN NW LED. The emission light intensity and injection current at a fixed applied voltage has been enhanced by a factor of 17 and 4 after applying a 0.093% compressive strain, respectively. Then, we extend the single NW device to NW LEDs array, for pressure/force sensor arrays for mapping strain with a resolution as high as 2.7 μm. Such sensors are capable of recording spatial profiles of pressure distribution, and the tactile pixel area density of our device array is $6250000/cm^2$, which is much higher than the number of tactile sensors in recent reports ($6\text{-}27/cm^2$) and mechanoreceptors embedded in the human fingertip skins ($240/cm^2$). This research may be a great step toward digital imaging of mechanical signals using optical means, having potential applications in artificial skin, touch pad technology, personalized signatures, bio-imaging and optical MEMS, and even and smart skin.

Invited Talk SYCO 1.5 Mon 12:00 H1

Bulk and Flexo-photovoltaic effect — •Marin Alexe, Ming-Min Yang, and Dong-Jik Kim — University of Warwick, Department of Physics, CV4 7AL Coventry, UK

Two years after the invention of modern prototype solar cells, it was found that a ferroelectric material exhibits a photovoltaic effect distinct from that of p-n junctions, later called the bulk photovoltaic (BPV) effect. Under uniform illumination, a homogeneous ferroelectric material gives rise to a current under zero bias, i.e. short-circuit current, that depends on the polarization state of the incident light and produces an anomalously large photo-voltage well exceeding the bandgap energy. The present talk will firstly present the basics of the bulk photovoltaic effect and the electronic origin of the anomalous BPV in multiferroic BiFeO3. I will finally discuss a new mechanically-induced photovoltaic effect [1] which turns the BPV effect into a universal effect allowed in all semiconductors by mediation of the flexoelectric effect.

[1] M. Yang, D.J. Kim, M. Alexe, Flexo-photovoltaic effect, Science 360, 904 (2018)