

## KFM 2: Microstructure of Thin Films / Crystal Structure

Chair: Enrico Langer (Technische Universität Dresden)

Time: Monday 9:30–11:10

Location: PHY 5.0.20

KFM 2.1 Mon 9:30 PHY 5.0.20

**Structural modification of thin Bi(1 1 1) films by passivation and native oxide model** — •CHRISTIAN KÖNIG<sup>1</sup>, STEPHEN FAHY<sup>1,2</sup>, and JAMES C. GREER<sup>3</sup> — <sup>1</sup>Tyndall National Institute, University College Cork, Lee Maltings, Cork T12 R5CP, Ireland — <sup>2</sup>Department of Physics, University College Cork, College Road, Cork T12 K8AF, Ireland — <sup>3</sup>Nottingham Ningbo New Material Institute and Department of Electrical and Electronic Engineering, University of Nottingham Ningbo China, 199 Taikang East Road, Ningbo, 315100, China

Bismuth is a promising material for electronic devices on the nanometer scale. Although the bulk material is semimetallic, a band gap can be expected in a thin film or nanowire due to quantum confinement. We investigated the structure of thin Bi(1 1 1) films with a thickness of approximately 1 nm with density functional theory. In order to remove metallic surface states, a passivation of the devices is necessary. Our calculations show considerable interaction of the surface with passivants like hydrogen and hydroxyl. The orientation of the thin films is changed completely whereas thick films are only affected at the surface. As the electronic properties of the material depend on the crystal structure, this effect is detrimental for device performance. Furthermore, we present model structures for the native oxide which form a protective capping layer and interact only weakly with the film so that the crystal orientation remains unchanged.

KFM 2.2 Mon 9:50 PHY 5.0.20

**Introducing Caesar: Ab Initio Modelling of the Properties of Materials over Large Temperature Ranges** — •MARK JOHNSON and RICHARD NEEDS — Theory of Condensed Matter, Cavendish Laboratory, University of Cambridge, United Kingdom

Caesar is a new code which is capable of modelling crystalline materials across most of the temperature range at which they remain crystalline. Caesar aims to provide calculations at ab initio accuracies whilst being fast enough, and autonomous enough, to be used as part of high-throughput methods such as structure searching.

Caesar can be interfaced with any electronic structure code, which is used as an engine to map out the nuclear energy landscape under the Born-Oppenheimer approximation. Nuclear motion in this landscape is modelled under the formalism of coupled anharmonic phonons, using vibrational self-consistent field theory and related methods. This allows for behaviour over a range of temperatures to be calculated from a single mapping of the energy landscape, and for the simulation of materials which are dynamically unstable under the harmonic approximation.

This talk will highlight advances to vibrational methods made in the development of Caesar, focussing on the exploitation of symmetry to accelerate the calculation and improve its accuracy. The talk will also present an overview of the current and future applications of the code, including work employing CASTEP as the engine used to predict the phase diagrams of elemental systems from first principles.

Break 20 min

KFM 2.3 Mon 10:30 PHY 5.0.20

**Time-resolved X-ray absorption spectroscopy on Al-Cu alloys – from solute copper to stable precipitates** — DANNY PETSCHKE, FRANK LOTTER, ELISCHA BLAESS, and •TORSTEN E.M. STAAB — University Wuerzburg, Dep. of Chemistry, LCTM, Roentgenring 11, D-97070 Wuerzburg, Germany

Although binary aluminium alloys seem to be uninteresting and well known, some aspects of their precipitation sequence – especially the early stages immediately after quenching – are still not well understood. Since the Al-Cu system is the basis for many ternary and quaternary high-strength alloys with application in the aviation sector, it is important to understand this binary system in detail. This problem is here tackled by a unique combination of differential scanning calorimetry and X-ray absorption fine structure measurements, where relaxed atomic coordinates for simulation of the spectra have been obtained by ab initio calculations. Thereby, it is possible to attribute any exo- or endothermic peak to a certain type of precipitate, even though formation and dissolution regions have a large overlap in this system. This unique combination of experimental and numerical methods allows one to determine the local atomic environment around Cu atoms, thus following the formation and growth of Guinier-Preston zones, i.e. Cu platelets on {100} planes, during the precipitation process.

KFM 2.4 Mon 10:50 PHY 5.0.20

**Distinctive bond breaking in crystalline phase-change materials and fingerprints for metavalent bonding** — •STEFAN MAIER<sup>1</sup>, OANA COJOCARU-MIRÉDIN<sup>1</sup>, MIN ZHU<sup>1</sup>, ANTONIO MIO<sup>1</sup>, JENS KEUTGEN<sup>1</sup>, MICHAEL KÜPERS<sup>2</sup>, YUAN YU<sup>1</sup>, JU-YOUNG CHO<sup>1</sup>, RICHARD DRONSKOWSKI<sup>2</sup>, and MATTHIAS WUTTIG<sup>1,3</sup> — <sup>1</sup>I. Institute of Physics (IA), RWTH Aachen University, 52074 Aachen, Germany — <sup>2</sup>Institute of Inorganic Chemistry, RWTH Aachen University, 52056 Aachen, Germany — <sup>3</sup>JARA-FIT Institute Green-IT, RWTH Aachen University and Forschungszentrum Jülich, 52056 Aachen, Germany

The field evaporation of a number of crystalline and amorphous phase-change materials and other intermetallic compounds was studied by laser-assisted atom probe tomography. A high probability of multiple detector events (i.e. more than one ion detected per laser pulse) was found for the crystalline materials. Amorphous phase-change materials and other materials showing classical metallic or covalent bonding, exhibit low probabilities. This unusual field evaporation is unlike any other known mechanism to result in high probabilities for multiple detector events. Hence, in the presented examples, laser-assisted field evaporation reveals striking differences in bond breaking. This is indicative for pronounced differences in the bonding mechanism (which we call metavalent bonding) and it implies the presence of chemical bonds, which differ significantly from classical covalent, ionic and metallic bonds. This is supported by other fingerprints, which are sensitive towards chemical bonding such as the optical dielectric constant.