MM 37: Microstructure and Phase Transformations

Transformation investigations by diffraction and imaging (TEM, XRD)

Time: Wednesday 11:45–13:00 Location: TC 010

MM 37.1 Wed 11:45 TC 010

X-Ray Studies of Large Crystals with Small Holes: The Case of Virtual Nanoporous Gold — •Bao-Nam Dinh Ngô[1], Matthias Graf[2], Jörg Weissmüller[1,2], and Jürgen Markmann[1,2] — [1]Institute of Materials Research, Materials Mechanics, Helmholtz-Zentrum Geesthacht, Geesthacht, Germany — [2]Institute of Materials Physics and Technology, Hamburg University of Technology, Hamburg, Germany

Nanoporous gold (NPG) made by dealloying is a polycrystalline material with 10 – 100 μm sized crystallites that are interpenetrated by a network of 10 – 100 nm sized pores. X-ray powder diffraction by such structures has not been systematically studied so far. We explore the issue by theory, experiment, and virtual diffraction, with an eye on establishing a method for nondestructive microstructure characterization of NPG. Virtual diffraction studied a computer-generated NPG sample with crystal size 61 nm and ligament size 4 nm. The diffraction pattern of the truncated (porous) periodic crystal lattice in its unrelaxed state agrees well with our theory: A narrow central component of the Bragg reflections reflects the long-range lattice coherency while a broad foot reflects the loss of atomic neighbors due to nanopores. Thermal relaxation using molecular dynamics leads to a complete loss of the narrow component. This can be attributed to crystal lattice distortion (microstrain) due to surface stress. The virtual diffraction is in excellent agreement with experimental diffraction data.

MM 37.2 Wed 12:00 TC 010

Effect of Ca substitution on structural, dielectric and optical properties of Ba5NdTi3Nb7O30 ceramic — Vipin Kumar[1], Satender Nath Pandey[2], and •Sardool Singh Ghumman[1] — [1]Physics department, Sant Longowal Institute of Engineering & Technology, Deemed University, Longowal, District Sangrur Punjab 148 106 India — [2]Physics Department, Motilal Nehru National Institute of Technology, Allahabad 211 004 India

The polycrystalline samples of pure Ba5NdTi3Nb7O30 and Ca substituted Ba4CaNdTi3Nb7O30, in the tetragonal tungsten bronze (TTB) family, are prepared by solid state reaction method. Formation of single phase of the complex compound of orthorhombic type has been verified by X-ray diffraction analysis in both the cases. Surface morphology and uniform growth of grains are examined by scanning electron microscopy. The dielectric properties as a function of frequency and temperature demonstrate dielectric anomaly of ferroelectric to paraelectric phase transition with raised Curie temperature at 107 oC in comparison to 100 oC of calcium free compound. Optical absorption spectrum with FTIR indicates red shift in M-O absorption bond which signifies the distortion in the lattice. The enhanced dielectric stability over a considerable range of temperature calls for the calcium doped material for use in devices on low frequency and high temperature operation.

MM 37.3 Wed 12:15 TC 010

Atomic scale structural transitions at stacking faults in C14 Fe2Nb Laves Phase — •Christian Liebscher[1], Michaela Šlapáková[1,2], Sharvan Kumar[3], and Frank Stein[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, 40237 Düsseldorf, Germany — [2]Charles University, Department of Physics of Materials, 12116 Prague, Czech Republic — [3]Brown University, School of Engineering, Providence, RI 02912, USA

Laves phases belong to the group of tetrahedrally closed-packed phases (TCP) and are commonly observed to exist in many material systems. The complex crystal structure of the C14 Fe2Nb Laves phase can be described by a layered arrangement of small (Fe) and large (Nb) atoms forming interpenetrating single and triple layers. By combining aberration-corrected scanning transmission electron microscopy (STEM) with atomic scale chemical spectroscopy, we unravel composition-induced atomic scale structural transitions at stacking faults in a Nb-rich Fe2Nb Laves phase. The fault density is observed to significantly increase with the presence of excess Nb atoms. Two basic variants, confined and highly extended faults are present. In the case of basal faults extending over several micrometers, nanometer-thin layers of the Fe7Nb6-phase are observed to form by the intercalation of multiple three-layer stacks of Nb atoms into the host Laves structure. At confined basal stacking faults, the formation of a fragmentary Fe7Nb6-phase is established, where a complete Fe kagomé layer is absent. This complexion is stablized by the imposed elastic and compositional constraints at the stacking fault.

MM 37.4 Wed 12:30 TC 010

Oxide texture as cause and effect in the corrosion of zirconium fuel cladding - an atomistic simulation and electron microscopy study — •Maria S Yankova, Felicity Baxter, Alistair Garner, Philipp Frankel, and Christopher P Race — School of Materials, University of Manchester, UK

Oxidation of the Zr alloy fuel cladding in light water reactors is one of the key degradation mechanisms, limiting the amount of fuel burned. The structural and electronic properties of monoclinic and tetragonal zirconia grain boundaries strongly affect the transport of species through the oxide layer. Hence, changes in oxide texture and phase fractions under irradiation can significantly alter the oxidation kinetics. We are exploiting a combination of density functional theory (DFT) simulation, scanning precession electron diffraction in the transmission electron microscope (TEM) and novel Python-based texture analysis to obtain an improved mechanistic understanding of the oxide microstructure. We have performed DFT calculations of the stiffness of key lattice planes in bulk zirconia to explore the effect of transformational stresses on the growth of grain orientations strongly represented in our experimental texture maps. We have revealed a correlation between the metal-oxide interface and a preferred texture orientation previously hidden by conventional texture analysis. We have investigated the effect of irradiation-induced defects and alloying elements on the structural and electronic properties of representative oxide grain boundaries using DFT and have identified the dominant point defects that control the oxide growth in an electrochemical environment.

MM 37.5 Wed 12:45 TC 010

Dynamics of sub-nm Pt clusters on carbon-based materials: Computation meets STEM measurements — Marta Bon, Trond Henninen, Daniele Passerone, and •Rolf Erni — Empa Swiss Federal Laboratories for Materials Science and Technology, Switzerland

Crystallization, condensation and precipitation from a solution are three different phase transitions which are commonly described by the classical nucleation theory (CNT). CNT is generally in agreement with experiments, however does not define what fundamentally constitutes a pre-nucleation state or how a nucleus is formed at all. State-of-the-art scanning transmission electron microscopy (STEM) allows observing the dynamics of clusters smaller than 2 nm in size at atomic resolution.[1] Being however 2D projections of the 3D geometry of the clusters, STEM images are challenging to interpret directly. Molecular dynamics simulations boosted by enhanced sampling techniques, such as metadynamics,[2] can complement the high-resolution STEM measurements, and shed light on the formation, dynamics, stability, and evolution of tiniest atomic clusters which represent the embryos of solid matter. We show, in particular, the Pt 3D structures deposited on carbon-based materials, explaining how temperature and the interactions between the Pt atoms and the substrate can affect the clustering process.

[1] T. J. Woehl, et al. ACS Nano 6.10 (2012): 8599-8610. [2] A. Barducci, G. Bussi, and M. Parrinello. Phys. Rev. Lett. 100.2 (2008): 020603.