MM 27.4 Wed 12:15 IFW B

3D Vertex Dynamics Simulation of Grain Growth in Ceramics Including the Anisotropy of Grain Boundary Energy — •Melanie Syha[1], Ling Yue[1], Daniel Weygand[1], and Peter Gumbsch[1,2] — [1]Universität Karlsruhe, Institut für Zuverlässigkeit von Bauteilen und Systemen — [2]Fraunhofer IWM, Freiburg

A three dimensional (3D) vertex dynamics model for grain growth is presented, adapted to the study of grain growth in Strontium-Titanate-Oxide (STO) ceramics. The 3D vertex dynamics model for grain growth is an interface tracking model [1]. In this approach grain boundaries (GB) are discretized and their time evolution is derived from the minimization of the GB energy, which is dissipated by the motion of the GBs and triple lines. The original model [1,2] has been extended to handle misorientation and inclination dependent GB energies, mobilities and triple line drag. The improved model is compared to the 3D analogue of the Neumann-Mullins law [3].

The influence of structure dependent GB properties on statistical observables, e.g. grain size distribution function, grain growth dynamics and correlation function between grain size and number of neighboring grains is investigated. Cross sections through the grain structures are analyzed and compared to experimental observations on grain growth in STO ceramics

[1] D. Weygand, Y. Bréchet, J. Lépinoux, and W. Gust, Phil. Mag. B 79 (1999) 703. [2] D. Weygand, Y. Bréchet and J. Lépinoux, Interface Science 7 (1999) 285. [3] R. MacPherson and D. Srolovitz, Nature 446 (2007) 1053

MM 27.5 Wed 12:30 IFW B

THE FINITE MOBILITY OF THE BOUNDARY JUNCTIONS AND THE THEORETICAL PREDICTIONS OF GROWTH RATE FOR POLYCRYSTALS UNDERGOING GRAIN GROWTH — •Luis Barrales-Mora — Institut für Metallkunde und Metallphysik, RWTH-Aachen, Aachen, Germany

As a consequence of the recent demonstration of the three-dimensional von Neumann-Mullins relationship by MacPherson and Srolovitz, there has been a renewed interest in the investigation of the phenomenon known as grain growth. This interest arises from the many possibilities that this new relationship offers but also, and contradictorily, from its limitations. One of such limitations is the impossibility of this relationship to predict correctly the volume rate of change of grains if the motion of the grain boundaries is hindered. It is well known that many factors can hinder the grain boundary motion, e.g., second-phase particles, impurity atoms, the finite mobility of the boundary junctions, etc. In the present contribution, the latter factor is analysed in light of the Cahn-MacPherson-Srolovitz relationship by means of computer simulations. This relationship is coupled with theories on the finite mobility of triple lines and quadruple junctions and compared with simulation results in single grains. Similar relationships by Glicksman and Rios and Hilgenfeldt et al. are also investigated. This last point is relevant since these approaches allow the study of grain growth from a more statistical point of view.

MM 28: Electronic Properties I

Time: Wednesday 10:15–11:45 Location: IFW D

MM 28.1 Wed 10:15 IFW D

The Tuneable Electron Mobility in Charged Indium Tin Oxide Thin Films — •Subho Dasgupta, Maya Lukas, Robert Kruk, and Horst Hahn — Institute for Nanotechnology, Forschungszentrum Karlsruhe GmbH, P.O. Box 3640, D-76021 Karlsruhe, Germany

This study aims at the quantitative understanding of the change in electronic transport upon surface charging in nanoparticulate and nanocrystalline conducting oxide. Previously, we demonstrated a device with a metallic conducting channel made of Indium Tin Oxide (ITO) nanoparticles which exhibits an on/off ratio of 2×10^3 [1]. To find the mechanism of such a large change in conductivity, we prepared nanocrystalline ITO thin films of a few nanometers thickness as a model system. It was observed that an increase in the Sn-doping level near the grain boundaries results in a local variation in the screening length upon charging. This variation is considered to be equivalent to an increase in the surface roughness resulting in the disruption of the conducting paths. It is concluded that primarily a change in the scattering probability is causing the high value of variation in transport properties for highly-doped semiconductors like ITO.

[1] S. Dasgupta, S. Gottschalk, R. Kruk, H. Hahn, Nanotechnology 19 (2008) 435203

MM 28.2 Wed 10:30 IFW D

The electrical properties of anodically oxidized Ti based NWFETS and its oxygen sensor applications — •Dawit Gedamu, Seid Jebril, Arnim Schuchardt, and Rainer Adelung — Functional Nanomaterials, Institute of Materials Science, Faculty of Engineering, CAU Kiel

A number of techniques have been reported on fabrication of tunnel junction nano structures through anodization in the last decade , . The dimension of such structures can be miniaturized and controlled through the anodic voltage while anodizing. A TiO2 tunnel junction of controlled thickness is similarly produced through anodic oxidation of Ti nanowires produced in a fracture approach . By using an electrochemically grown TiO2 as a gate oxide, we demonstrate nanowire field effect transistors (NWFET) which can be further used as oxygen sensor. Although FET based sensors are undoubtedly of great importance for microelectronics smart sensors, there are limited sensor reports on FET sensor. Gas detection based on this technique relies largely on change of the metal work function in the Schottky diode or MOSFETs induced by catalytic reaction on the solid surface . Here, the oxygen sensing properties are also demonstrated.

MM 28.3 Wed 10:45 IFW D

Phonon absorption at low temperature - determination of the indirect band gap in FeSi using Fourier-spectroscopic infrared ellipsometry — •Dirk Menzel[1], Paul Popovich[2], Alexander V. Boris[2], and Joachim Schoenes[1] — [1]Institut für Physik der Kondensierten Materie, TU Braunschweig, Germany — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

The determination of the band gap is an important parameter for the characteristics of a semiconductor. However, for FeSi the size of the gap is not reported consistently so far. Using far-infrared spectroscopic ellipsometry we have reliably determined the dielectric function of FeSi. As predicted by band structure calculations both a direct and an indirect band gap are observed from the absorptive part of the dielectric function which amount to 73 meV and 10 meV, respectively. The absolute value of the indirect gap can only be evaluated when both phonon absorption and emission are observed. At low temperature, however, the former does not occur which generally makes it impossible to obtain the indirect gap energy in the low temperature range. For the ellipsometric measurements we used a Fourier transform spectrometer and, therefore, illuminated the sample with white light. This leads to a continuous generation of optical phonons which may also decay into low-energy acoustic phonons. This method enables one to derive the absolute value of the indirect gap even the low temperature.

MM 28.4 Wed 11:00 IFW D

$Co_xFe_{(x-1)}S_2$: How close to half-metallicity? — •C. Utfeld[1], S. R. Giblin[2], J. W. Taylor[2], J. Laverock[1], S. B. Dugdale[1], C. Shenton-Taylor[3], J. A. Duffy[3], L. Wang[4], C. Leighton[4], M. Itou[5], and Y. Sakurai[5] — [1]H.H. Wills Physics Laboratory, University of Bristol, Tyndall Avenue, Bristol BS8 1TL, UK — [2]ISIS Facility, RAL, Chilton, Oxfordshire OX11 0QX, UK — [3]Department of Physics, University of Warwick, Coventry CV4 7AL, UK — [4]Chem. Eng. & Mat. Sci., University of Minnesota, Minneapolis, MN 55455, USA — [5]SPring-8, 1-1-1 Kouto, Mikazuki, Sayo, Hyogo 679-5198, Japan

CoS_2 is a material thought to be very close to being a half-metal, i.e. to only be conducting in one spin. However, the Fermi level lies low in the conduction bands and doping with the isostructural semiconductor FeS_2 is predicted to gradually unoccupy one spin channel. In this context the evolution of the polarisation across the series $Co_xFe_{(1-x)}S_2$ is of major interest. Experimentally the number of direct measurements accessing the bulk polarisation for different alloy compositions is rather