MM 56: Topical Session Growth Kinetics VI

Time: Thursday 15:30–17:00 Location: H4

MM 56.1 Thu 15:30 H4

Computational analysis of interfacial attachment kinetics and transport phenomena during liquid phase epitaxy of mercury cadmium telluride — Igal Rasin[1], Anne Ben Dov[2], Ilana Grimberg[2], Olga Klin[2], Eliezer Weiss[2], and •Simon Brandon[1] — [1]Dept. of Chemical Engineering, Technion, Haifa 32000, Israel — [2]SCD-Semi-Conductor Devices, P.O. Box 2250/99, Haifa 31021, Israel

Deposition of mercury cadmium telluride (MCT) thin films, on lattice matched cadmium zinc telluride substrates, is often achieved via Liquid Phase Epitaxy (LPE). The yield and quality of these films, required for the production of infrared detector devices, is to a large extent limited by lack of knowledge regarding details of physical phenomena underlying the deposition process. Improving the understanding of these phenomena and their impact on the quality of the resultant films is therefore an important goal which can be achieved through relevant computational and/or experimental studies.

We present a combined computational and experimental effort aimed at elucidating physical phenomena underlying the LPE of MCT via a slider growth process. The focus of the presentation will be results generated by a time-dependent three-dimensional model of mass transport, fluid flow, and interfacial attachment kinetics, which we have developed and applied in the analysis of this LPE process. These results, combined with experimental analyses, lead to an improved understanding of the role of different transport and kinetic phenomena underlying this growth process.

MM 56.2 Thu 15:45 H4

Zeolite thin film growth studied with a phase-field model — •Frank Wendler, Christian Mennerich, and Britta Nestler — Institute of Materials and Processes, Karlsruhe University of Applied Sciences, Moltkestr 30, 76133 Karlsruhe, Germany

Hydrothermally grown zeolite films are exeptionally interesting as molecular sieves, where the transport through the nanosized pores is strongly modulated by the grain orientation and boundary morphology. The objective of the simulation study is an understanding of the competitive growth behaviour and the formation of undesired mesoscale porosity during polycystalline growth to optimize process conditions. We adopt a multi-phase field model of Allen-Cahn type to describe the process, where each solid grain and the aquaeous solution are represented by individual order parameters. First, single coffin- or leaflet-shaped MFI zeolite crystals are modeled choosing appropriate anisotropies of surface tension and kinetic coefficient. Different aspect ratios and a transition between both crystal growth shapes emerge. Then, the selection dynamics is studied in simulations with several hundreds of grains in 2D and 3D, showing a gradual extinction according to misorientation and the influence of non-isotropic orientation distributions (seeded growth). The occurence and influence of growth twinning on the morphological evolution is discussed, which - similar to nucleation - produces new growth orientations during the process. Parts of the complex silicate chemistry are represented by taking into account the initially present gel phase (solution + amorphous solid), acting as a buffer layer in the transport of the silicate building blocks.

MM 56.3 Thu 16:00 H4

Combined phase-field and MD simulations of diffusion drop and ordering at $[Ni_xZr_{1-x}]_{liquid}$-$Zr_{crystal}$ interfaces — •M. Guerdane, F. Wendler, and B. Nestler — Institute of Materials and Processes, Karlsruhe University of applied Sciences, Germany

We combine phase-field (PF) modeling and molecular dynamics (MD) simulations to show that the velocity of the solidification front in a two-phase $[Ni_xZr_{1-x}]_{liquid}$-$Zr_{crystal}$ structure is strongly affected by the drop of the liquid diffusion when approaching the solid-liquid interface. The latter is defined through a suitable order parameter that distinguishes between crystalline and liquid atomic environment. The diffusion drop near the interface is attributed to the pronounced short range order inherent to the Ni_xZr_{1-x} melt. The system transforms into a massive lateral ordering in the vicinity of the Zr crystalline wall. Our combined PF-MD analysis points out the shortcoming of the standard interpolation procedure, usually applied in constructing the phase dependent diffusivity, to describe the confinement effect caused by the crystalline wall at low temperatures.

MM 56.4 Thu 16:15 H4

The Interface of a Growing Zr-Ni Crystal — •Philipp Kuhn and Jürgen Horbach — Deutsches Zentrum für Luft- und Raumfahrt, Institut für Materialphysik im Weltraum, Köln

Crystal growth of intermetallic phases in binary metallic alloys proceeds at a considerably slower pace than that of pure metals. As an example the growth in Zr-Ni is two orders of magnitude slower than that for pure Ni [1]. We perform molecular dynamics simulations of pure Ni and Zr-Ni systems to elucidate the mechanism behind this phenomenon. As an interaction model an embedded atom potential is used [2]. We utilize local order parameters to distinguish between solid and liquid particles and combine them in the form of two-dimensional maps [3] as a tool to analyze the structure of the layers in the interface region. This analysis serves as a prerequisite to determine the kinetics of mass transport in the interface region.

[1] H. Yasuda et al., J. Phys. **144**, 012056 (2009)

[2] T. Kumagai et al., Mat. Transact. **48** Nr. 6, pp. 1313–1321 (2007)

[3] W. Lechner and C. Dellago, J. Chem. Phys. **129**, 114707 (2008)

MM 56.5 Thu 16:30 H4

Conditions for the occurrence of Abnormal Grain Growth studied by a 3D Vertex Dynamics Model — •Melanie Syha and Daniel Weygand — KIT, Institut für Zuverlässigkeit von Bauteilen und Systemen, Kaiserstr. 12, 76128 Karlsruhe

The three dimensional (3D) vertex dynamics model presented in [1,2] has proven to be suited to model the coarsening of systems of up to several thousand grains with an excellent agreement to the MacPherson/Srolovitz relation for the volume change rate. Now this model is applied to investigate the phenomenon of Abnormal Grain Growth (AGG) in SrTiO3.Although the effect of AGG in perovskite materials in absence of pinning is covered by several investigations [3,4] the underlying mechanisms are still not well understood.In contrast to classical mean field approaches which often assume special but uniform GB properties for the abnormally growing grain of size r, the present study focusses on the role of GB mobility and energy variation, such as inclination dependencies, on the onset of AGG. [1] M. Syha, D. Weygand, A generalized vertex dynamics model for grain growth in three dimensions, accepted for publication, Modeling Simul. Mater. Sci. Eng. [2] D. Weygand, Y. Bréchet, J. Lépinoux, W. Gust, Three dimensional grain growth: A vertex dynamics simulation,Phil. Mag. B 79 (1999) 703-16 [3] T. Sano, G. Rohrer, Experimental evidence for the Development of Bimodal Grain Size Distributions by the Nucleation-Limited Coarsening Mechanism, J. Am. Ceram. Soc. 90 (2007) 199-204 [4] C. Bae, J. Park, Y. Kim, H. Jeon, Abnormal Grain Growth of Niobium-Doped Strontium Titanate, J. Am. Ceram. Soc. 81 (1998) 3005-09

MM 56.6 Thu 16:45 H4

Twist grain boundary migration by molecular dynamics simulation — •Volker Mohles, Jian Zhou, and Günter Gottstein — Institute of Physical Metallurgy and Metal Physics, RWTH Aachen University, Aachen, Germany

Molecular dynamics (MD) simulations with EAM potentials were used to study grain boundary migration of [001], [110] and [111] twist grain boundaries (GBs) in aluminum. The motion of GBs was driven by a crystal orientation dependent driving force. During GB migration, all GBs were found to be flat and to retain their structures at a given temperature. The GB structure was found to vary depending on temperature and the misorientation angle, and to be crucial for GB mobility. For some high-angle high-energy GBs, a transition from a solid-like structure to a liquid-like one was observed at elevated temperatures. This transition affects GB migration significantly. Our simulations yield twist GB mobility data in conspicuous agreement with those derived from real experiments.