MM 55: Topical Session Growth Kinetics V

Time: Thursday 14:00–15:15 Location: H4

MM 55.1 Thu 14:00 H4

Atomic scale simulations of silicon growth from the melt: Formation of twins and stacking faults studied by molecular dynamics and Monte Carlo methods — •Johan Pohl and Karsten Albe — Institut für Materialwissenschaft, TU Darmstadt, Petersenstr. 32, D-64287 Darmstadt

Formation of twin boundaries and stacking faults at the silicon growth front is studied by lattice Monte Carlo and molecular dynamics (MD) simulations. First, we show how to construct a computationally efficient lattice-based Monte Carlo model that includes stacking faults and twin boundaries and allows to simulate crystal growth of large systems. Data on the importance of stacking faults for the roughening transition of the (111) interface and parallel twin growth velocities are extracted from the model.

In a further step, MD simulations reveal that twins do not nucleate on (111) microfacets in the perfect crystal, but exclusively occur in the vicinity of grain boundaries [1]. Only at an undercooling of 150 K we observe the formation of metastable twin bounded loops with incoherent interfaces to the matrix consisting of coherency and anticoherency dislocations. We conclude that the nucleation of stable twins in silicon growth requires the presence of a grain boundary or more general of a three-phase boundary, but is unlikely to occur on ideal (111) facets because of the excess energy of the interfacial area between matrix and twinned crystal.

MM 55.2 Thu 14:15 H4

Nutzung der Wachstumskinetik in Wandermagnetfeldern für die Czochralski-Züchtung von PV-Silizium mit quadratischem Querschnitt — •P. Rudolph[1], M. Czupalla[1], B. Lux[1] und F. Kirscht[2] — [1]Leibniz-Institut für Kristallzüchtung (IKZ), Berlin — [2]CaliSolar GmbH, Berlin

Bei der Herstellung von Si-Solarzellen mit Standardkantenlängen von 125 bzw. 150 mm aus den zylindrischen Czochralski-Kristallen entstehen Präparationsverluste von 25-28%. Von Vorteil wäre das Ziehen von CZ-Kristallen mit quadratischem Querschnitt. Um die Verwendung kontaminierender Formgeber zu umgehen, kann man sich die kinetisch determinierte Ausbildung von seitenbegrenzenden Wachstumsfacetten zunutze machen. Wenn es gelingt sehr geringe radiale und zudem stabile Temperaturgradienten über den Tiegelradius einzustellen, wird der in [001]-Richtung gezogene Si-Kristall von vier {110}-Seitenflächen begrenzt. Nach Brice ist in einem konzentrischen Isothermenfeld die Facettenbreite $d = (2\Delta T R/G_T)^{1/2}$ mit R - Radius der Schmelzpunktisotherme, G_T - senkrecht dazu verlaufendem radialen Temperaturgradienten und ΔT - die für eine 2D-Keimbildung im Facettenzentrum erforderliche Unterkühlung. Mit einer spezifischen Heizer-Magnet-Konfiguration wird ein magnetisches Wanderfeld erzeugt, welches eine sehr stabile toroidale Strömung in der Schmelze mit extrem geringem G_T generiert. Bisher konnten reproduzierbar Si-Einkristalle solcher Querschnitte mit Kantenbreiten $d = 50 - 90$ mm gezogen werden. Strukturelle Perfektion, Sauerstoffgehalt und mikroskopische Morphologie der {110}-Facetten werden analysiert.

MM 55.3 Thu 14:30 H4

Minimum Energy Path for Nucleation with Phase Field Crystal — •Axel Voigt and Rainer Backofen — TU Dresden

Phase Field Crystal (PFC) is a well established model to study solidification in metals and colloids on an atomistic scale [1,2]. It can be connected to time dependent classical density functional theory. The time evolution of the density of particles is governed by a (at least) 6-th order partial differential equation. Thus, it is straight forward to calculate the time evolution of states, which is a minimization of total energy in the system. But, in order to study nucleation, the transition path between two (meta) stable states has to be explored. The nucleation barrier is then defined by the most probable transition path. This is equivalent to the minimum energy path (MEP). The MEP is the path in configuration space, where the driving force or dynamics of the system is parallel to the transition path [3]. Thus, the MEP allows us to identify saddle points which has to be overcome by nucleation as well as nucleation barriers. Recently a simplified string method was proposed in order to calculate MEP in high dimensional configuration spaces [3]. We will show the application of the simplified string method to nucleation in phase field crystal. Nucleation barriers as well as morphology of minimal stable nuclei will be discussed. Furthermore the influence of walls to nucleation will be shown.

[1] S. van Teeffelen, R. Backofen, A. Voigt and H. Loewen, Phys. Rev. E 79 051404 (2009) [2] R. Backofen, A. Raetz and A. Voigt, Phil. Mag. Let. 87 (11),(2007) [3] W. E, W. Ren and E. Vanden-Eijnden, J Chem. Phys. 126, 164103 (2007)

MM 55.4 Thu 14:45 H4

Role of Nucleation in Multi-Scale Phenomena of Solidification — •Abhik Choudhury and Britta Nestler — Institute of Materials and Processes, Moltkestrasse 30, Karlsruhe 76131

Solidification has been an interesting topic of study considering the vast scale of structures possible during the evolution of solids from an undercooled liquid. Considering their significance, it is worthwhile to get a basic understanding of the principles underlying the pattern formations, such that control mechanisms are possible to design their production. Epicentric are structures such as interdendritic lamellar eutectics and island banded and coupled growth morphologies in peritectic systems, which are principally formed as a result of interplaying multi-scale phenomena. Nucleation is understood to be an important phenomenon in maintaining scale of the eutectic lamellae in the case of interdendritic structures and the switching from island banded structures to coupled growth in some peritectic systems.

In the present study, we investigate the process of nucleation using the phase-field method. The presentation involves the calculation of the barrier to nucleation in eutectic and peritectic systems through the solution of the Euler-Lagrange(EL) equations which are formulated in the framework of the phase-field method. Special emphasis is placed on the description of a novel technique to solve the EL equations, based on an extension of the volume preservation method. The generality of the method allows for applications to a range of possible EL equations in material systems. The calculations are compared with phase-field simulations of nucleation with random noise.

MM 55.5 Thu 15:00 H4

Trapping effects on the critical nucleus size in nucleation a growth processes, kinetic Monte Carlo simulations — •Zoltan Balogh[1,2], Zoltan Erdelyi[2], and Dezso L Beke[2] — [1]Westfälische Wilhelms Universität-Münster, Institut für Materialphysik, Münster, Germany — [2]University of Debrecen, Department of Solid State Physics, Debrecen, Hungary

The critical nucleus size - above which a nucleus will grow and below dissolve - is calculated in a binary alloy during diffusion controlled phase separation using kinetic Monte Carlo simulations. In the calculations the differences in atomic mobilities are often neglected, however the difference of diffusion coefficients in a binary alloys can be as high as 4-8 orders of magnitude in technically important materials (like Si-Ge, Fe-Cr or Ni-Cu).

If the atomic jumps are slower in the A-rich nucleus than in the embedding B-rich matrix, the nucleus will trap the approaching A atoms to its surface. It has not enough time to reject them - despite this process would be favored thermodynamically - before new A atoms arrive. Thus the kinetic and thermodynamical critical size would be different for the nucleus. With reasonable trapping effect the former can be even an order of magnitude smaller than the latter.