DS 42: Layer Growth: Evolution of Structure and Simulation

Time: Friday 16:15–17:15 Location: H 2032

DS 42.1 Fri 16:15 H 2032

Numerical simulation of demixing of a binary mixture on the solid substrate with a free surface — •Lubor Frastia[1] and Len M. Pismen[2] — [1]MPG PKS, Nöthnitzer Straße 38, 01187 Dresden, Germany — [2]Dept. of Chemical Engineering, Technion, 32000 Haifa, Israel

The problem of simultaneous demixing and dewetting is frequently occuring in nano-technological applications, where the thickness of the internal interfaces in the phase-separated liquid may be comparable to the droplet size or layer thickness. Theoretical approaches to the demixing problem are commonly based on the Cahn–Hilliard theory [1] using the Landau–Cahn free energy functional approximation to model phase separation while neglecting the effects of the moving surfaces [2].

In this contribution, we describe the static limit of the model, given in [3], specialized for a 2D film lying on a solid substrate. Based on this model, we derived the Finite Element (FE) numerical procedure and computed droplet solutions for selected parameters of the model, using a continuation procedure with surface tension of the free surface, γ, as the continuation parameter. Resulting solution branch is compared with the related circular-symmetric droplet solution and its effective sharp interface approximation.

References:

1. J.W. Cahn and J.E. Hilliard, J. Chem. Phys. **28**, 258–267 (1958).

2. H.P. Fischer, P. Maass, and W. Dieterich, Europhys. Lett. **42**, 49–54 (1998).

3. U. Thiele, S. Madruga, L. Frastia, submitted to Physics of Fluids.

DS 42.2 Fri 16:30 H 2032

Molecular dynamics simulation study of the silicon carbide precipitation process — •Frank Zirkelbach[1], Jörg K. N. Lindner[1], Kai Nordlund[2], and Bernd Stritzker[1] — [1]Experimentalphysik IV, Institut für Physik, Universität Augsburg, Universitätsstr. 1, D-86135 Augsburg, Germany — [2]Accelerator Laboratory, Department of Physical Sciences, University of Helsinki, Pietari Kalmink. 2, 00014 Helsinki, Finland

The precipitation process of silicon carbide in heavily carbon doped silicon is not yet understood for the most part. High resolution transmission electron microscopy indicates that in a first step carbon atoms form C-Si dumbbells on regular Si lattice sites which agglomerate into large clusters. In a second step, when the cluster size reaches a radius of a few nm, the high interfacial energy due to the SiC/Si lattice misfit of almost 20A molecular dynamics simulation approach is used to gain information of the precipitation process on the atomic level. A newly parametrized Tersoff like bond-order potential is used to model the system appropriately. The present work discusses the first results gained by the molecular dynamics simulation.

DS 42.3 Fri 16:45 H 2032

Monitoring quantum dot growth by in-situ cantilever systems — •yan wang[1,2], huiling duan[1,2], and joerg weissmueller[1,3] — [1]Institute of Nanotechnology, Forschungszentrum Karlsruhe, Postbox 3640, Karlsruhe, 76021, Germany — [2]College of Engineering, Peking University, Beijing, 100871, P. R. China — [3]Technische Physik Universität des Saarlandes, 66041 Saarbruecken, Germany

There exist many theoretical and experimental works that focus on understanding the growth mechanisms of quantum dots (QDs). Without an in-situ measurement technique that monitors the growth modes of QDs such as the Frank-van der Merwe (FM), the Volmer-Weber (VW), the Stranski-Krastanow (SK) growth modes, and their corresponding ripening states during deposition, it is difficult to make conclusions on the growth mechanisms and on the ripening mechanisms of QDs. To monitor the growth modes, QDs are located on a MBE chamber equipped with an in-situ cantilever measurement setup, and this cantilever is used as a substrate of QD growth.

In this paper, based on continuum models, we investigate a series of problems related to the strained heteroepitaxial in-situ cantilever systems of QD growth.We first obtain the curvature of this cantilever system, which provides a way to monitor the possible growth modes (FM, VW, SK and their corresponding ripening states) in terms of island density, wetting layer thickness and cantilever thickness, etc. Then, we give the equilibrium conditions for SK growth, which provide the theoretical basis to control the sizes and the shapes of QDs. Finally, we simulate the morphological evolution of SK system.

DS 42.4 Fri 17:00 H 2032

Does ion beam divergence affect pattern formation by surface sputtering? — •Taha Yasseri[1], Emmanuel O. Yewande[2], Alexander K. Hartmann[3], and Reiner Kree[1] — [1]Institute for Theoretical Physics, University of Göttingen, Friedrich-Hund Platz 1, D-37075 Göttingen, Germany. — [2]Department of Computing and Mathematics, Manchester Metropolitan University, John Dalton Building, Chester Street, Manchester M1 5GD, United Kingdom — [3]Institut for Physics, University of Oldenburg, Carl-von-Ossietzky Strasse 9-11, 26111 Oldenburg, Germany.

In recent works on creating patterns like quantum dots or ripples via ion-beam surface sputtering, the importance of beam divergence for the creation of clear patterns is emphasized. Motivated by these experiments, we perform a (2+1)- dimensional Monte Carlo simulations of surface sputtering to study the influence of beam divergence on dynamics of pattern formation. We explain our results using linear continuum theory via evaluating the rate of growth for different modes. Generally beam divergence leads to a combination of different growth rates which slows down pattern formation. We find two exceptional situations where ion beam divergence may improve the quality of patterns. (1) Ion incidence perpendicular to the surface and (2) ion incidence around the critical angle where the orientation of formed ripples changes by 90 degrees. In case (1) anisotropic beam profiles with divergence may lead to ripples whereas isotropic profiles mainly affect the length scale of the formed dots. In case (2) non-zero beam divergence leads to patterns consisting of crossed ripples.