Rapid metal-sulphide-induced crystallization of highly textured tungsten disulphide thin films. — •Stephan Brunken[1], Rainald Mientus[2], and Klaus Ellmer[1] — [1]Hahn-Meitner-Institut, Glienicker Straße 100, 14109 Berlin — [2]Optotransmitter-Technologie-Umweltschutz e.V., Köpenicker Straße 325b, 12555 Berlin

Highly (001) textured tungsten disulphide (WS_2) thin films are grown by rapid metal(Co, Ni, Pd)-sulfide-induced crystallization of amorphous reactively sputtered sulphur-rich tungsten sulphide (WS_{3+x}) films. The rapid crystallization is monitored by real-time in-situ energy dispersive X-ray diffraction (EDXRD). Provided that a thin metal film is deposited prior the deposition of WS_{3+x} the films crystallize very fast (about 20 nm/s). The crystallization starts in the range of the Ni-S eutectic temperature of 637 °C. After crystallization isolated MeS(Me = Co, Ni, Pd)-crystallites are located on the surface of the WS_2-layer, which is proved by scanning electron microscopy and transmission electron microscopy. Taking into account the crystallization temperature this leads to the model of the rapid crystallization from liquid MeS_x droplets, which dissolve WS_x, oversaturate, release WS_2 while floating on the top of the crystallizing volume to the top of the layer. These metal-sulphide-induced crystallized $WS_2$2-layers exhibit a pronounced (001) orientation with large crystallites up to 3 μm. They show photoactivity and high hole mobilities (about 50 cm^2/Vs). Combined with the high absorption coefficient of 10^5 cm^{-1} and a direct band gap of 1.8 eV these properties make such films suitable for absorber layers in thin film solar cells.

DS 41.6 Fri 15:45 H 2032

Preparation of $CuInS_2$ chalcopyrite films by reactive magnetron sputtering: Influence of the Particle Energy on morphological, electrical and optical properties — •Stefan Seeger and Klaus Ellmer — Hahn-Meitner-Institut, Dep. Solar Energetics, Glienicker Str. 100, 14109 Berlin

Today magnetron sputtering is a common technique for large area depositions and already used to fabricate layers for thin film solar cells: the back contact (molybdenum) and front contact (zinc oxide) or for the deposition of metallic precursors. Nevertheless it is astonishing that this technique is not yet used for preparing the absorber layer in photovoltaic devices. Recently we have demonstrated that reactive magnetron sputtering from an indium and a copper target in an Ar/H_2S atmosphere is suited to prepare $CuInS_2$ absorber films and solar cells with an efficiency of more than 10% in a one-step process without additional annealing procedures. In order to make full use of the advantages of a plasma-assisted deposition process:
i) deposition at lower temperatures compared to pure thermal processes,
ii) high chemical reactivity,
iii) compact and well adherent films,
we have investigated in this work the influence of the particle energies on the film growth and the electronic properties.

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.