DS 40: Thin Film Properties: Structure, Morphology and Composition I

Time: Thursday 15:00–16:30 Location: CHE 89

DS 40.1 Thu 15:00 CHE 89

Novel Type of Bent-Lattice Nanostructure in Crystallizing Amorphous Films: from Transrotational Crystals to Amorphous Models — •Vladimir Kolosov — Ural Federal University, Ekaterinburg, Russia

Unusual transrotational thin crystals with curvilinear lattice [1] have been discovered by transmission electron microscopy (TEM) for crystal growth in thin (10-100 nm) amorphous films for growing number of different substances. The formation of unexpected transrotational nanostructures can be traced in situ in TEM column. Transrotation (unit cell translation is complicated by small rotation realized round an axis lying in the film plane) can result in strong regular lattice orientation gradients (up to 300 degrees per 1 micron) of different geometries: cylindrical, ellipsoidal, toroidal, saddle, etc. Complex skyrmion-like lattice orientation texture is observed in some spherulite crystals. The transrotation phenomenon is the basis for novel lattice-rotation/strain nanoengineering. Transrotational micro crystals have been eventually recognized in some vital thin film materials, i.e. PCMs for memory [2-3]. New nanocrystalline models of amorphous state are proposed: fine-grained structures with lattice curvature. Going to 3D clusters of positive/negative curvature and dynamics we propose the hypothesis of "dilatons" and "contractons" pulsating or/and circulating in amorphous/glassy solids. [1] V.Yu. Kolosov and A.R.Tholen, Acta Mat., 48 (2000) 1829. [2] B.J. Kooi and J.T.M. De Hosson, JAP, 95 (2004), 4714. [3] E. Rimini et al, JAP, 105 (2009), 123502.

DS 40.2 Thu 15:15 CHE 89

Evaluation of atomically-resolved high-resolution TEM images of Di-and Tri- Re molecules @ SWNT with convolutional neural networks — •Christopher Leist, Kecheng Cao, and Ute Kaiser — Central Facility of Electron Microscopy Materials Science, Ulm University, 89081 Ulm, Germany

Single-walled carbon nanotubes (SWNT) containing transition metal Di- and Tri- Re molecules are investigated using atomic resolution transmission electron microscopy (TEM).The images are taken at 80kV with the Cc/Cs-corrected SALVE instrument operated at 80kV, where the nanotube can be stable and sub-Angstrom resolution can be achieved. Detailed analysis of the Re atom distances is not only time consuming, also many interesting image features are close to the scale of the pixel error, and the manual evaluations are prone to user bias. Here we use deep learning routines which have the potential of both speeding up the evaluation process considerable as well as reducing the accompanied bias. The neural networks are trained on simulated TEM images. Here we present our progress in training the neural network and thereby automating the image investigation.

DS 40.3 Thu 15:30 CHE 89

Helium Ion Microscope (HIM) Imaging and Time-of-Flight Secondary Ion Mass Spectrometry (TOF-SIMS) depth profiling of sample cross sections — •Nico Klingner, René Heller, and Gregor Hlawacek — Helmholtz-Zentrum Dresden-Rossendorf, Institute of Ion Beam Physics and Materials Research, Bautzner Landstr. 400, 01328 Dresden, Germany

The HIM is well known for its high-resolution imaging and nanofabrication performance. We have recently developed and presented a time-of-flight secondary ion mass spectrometer that can be retrofitted to existing microscopes [1,2].

Depth profiling in SIMS in general is usually done by sputtering into deeper layers and plotting the signal intensity over time. The actual milling depth can only be estimated and the common approach is to measure the crater depth with atomic force microscopy every time a compositional change is observed.

Direct imaging and chemical analysis of a cross-section with high spatial resolution can avoid this challenge. The cross sections will be prepared ex-situ by milling, grinding and low energy argon ion polishing.

[1] Klingner, N.; Heller, R.; Hlawacek, G.; von Borany, J.; Notte, J. A.; Huang, J. and Facsko, S.; Ultramicroscopy 162(2016), 91-97

[2] Klingner, N.; Heller, R.; Hlawacek, G.; Facsko, S. and von Borany, J.; Ultramicroscopy 198(2019), 10-17

DS 40.4 Thu 15:45 CHE 89

Impurity-Enhanced Solid-State Amorphization and Its Influence on Thin Film Formation — •Koen van Stiphout — Instituut voor Kern- en Stralingsfysica, KU Leuven, 3001 Leuven, Belgium — 2nd Institute of Physics, Georg-August-University Göttingen, 37077 Göttingen, Germany

The growth of amorphous compound thin films at the interface between a metal film and a semiconductor substrate upon annealing, has been studied extensively in the past. However, little is known about the influence of impurities of such a *solid-state amorphization (SSA)* reaction. Using *in situ* techniques, including synchrotron X-ray diffraction (XRD) and Rutherford backscattering spectrometry (RBS), we show that when small amounts of nitrogen impurities ($<$ 2 at.%) are implanted under the right conditions, the amorphous, intermixed layer during the Ni-Si reaction can reach thicknesses of almost 70 nm before crystallizing, an order-of-magnitude thicker than in the unimplanted system[1]. The delayed crystallization of the amorphous layer has profound effects on the reaction path of the system, as the early stages of phase formation become an interplay of long-range diffusion and kinetic nucleation barriers. Furthermore, we show that the increased stability of the amorphous phase is not just a particularity of the solid-phase reaction, but a general property of the Ni-Si system. At the heart of this *impurity-enhanced* SSA reaction lies the strong asymmetry in atomic mobility of the elements, which is increased due to the addition of an immobile, insoluble impurity element.

[1] K. van Stiphout *et al.* 2019, J. Phys. D: Appl. Phys. **52**, 145301

DS 40.5 Thu 16:00 CHE 89

Band Engineering in Photonic Crystals with multi-order Square Lattice — •Jiaxu Chen, Fanzhou Lv, Yudie Huang, Zhihang Wang, Shiyao Jia, Yi Wang, and Wenxin wang — Harbin Engineering University, Harbin, China

2D Photonic crystals (PCs) can be artificially arranged as periodic arrays to arise interesting optical characteristics, because of their intrinsic photonic band structures that are obviously determined by the lattice parameters. Therefore, the idea of band engineering can be realized by nanofabrication and provides an effective way to control the optical performance. However, most studies focus on band engineering by embedding elements at high symmetry points (Γ, X, M) of Brillouin zone in reciprocal-space, systemic studies along the path (Δ, Σ, Z) between symmetry points are still lacking. Here, 2D PCs with square lattice are engineered into muti-order lattices by carefully embed with other periodic elements at specific positions that correspond embedding lattice sites at non-high-symmetry points of Brillouin zone. This work proves non-high-symmetry point embedding is also an approach for photonic band engineering in photonic crystals as well as high-symmetry point and it is an effective way to modulate the photonic performances. As a result, the engineered photonic bands of PCs exhibit Dirac-like conical dispersions and flat band structure.

DS 40.6 Thu 16:15 CHE 89

Band Engineering in Photonic Crystals with multi-order Square Lattice — •Chen jiaxu — Harbin Engineering University, Harbin, China

2D Photonic crystals (PCs) can be artificially arranged as periodic arrays to arise interesting optical characteristics, because of their intrinsic photonic band structures that are obviously determined by the lattice parameters. Therefore, the idea of band engineering can be realized by nanofabrication and provides an effective way to control the optical performance. However, most studies focus on band engineering by embedding elements at high symmetry points (Γ, X, M) of Brillouin zone in reciprocal-space, systemic studies along the path (Δ, Σ, Z) between symmetry points are still lacking. Here, 2D PCs with square lattice are engineered into muti-order lattices by carefully embed with other periodic elements at specific positions that correspond embedding lattice sites at non-high-symmetry points of Brillouin zone. This work proves non-high-symmetry point embedding is also an approach for photonic band engineering in photonic crystals as well as high-symmetry point and it is an effective way to modulate the photonic performances. As a result, the engineered photonic bands of PCs exhibit Dirac-like conical dispersions and flat band structure.