O 39: Phase transitions

Time: Tuesday 15:00–16:15 Location: H42

O 39.1 Tue 15:00 H42

On the phase transition behaviour of confined molecular assemblies: The influence of the crystal structure on the freezing-melting transition — •Sebastian Mörz[1], Christof Schäfer[1], Andriy Kityk[2], Klaus Knorr[1], and Patrick Huber[1] — [1]Technische Physik, Universität des Saarlandes, Saarbrücken, Germany — [2]Institute for Computer Science, Czestochowa University of Technology, Czestochowa, Poland

The phase transition behaviour of simple fluids is strongly altered when confined to a mesoporous sorbent. The formation of supercooled states during cooling gives rise to a pronounced hysteresis between freezing and melting of pore confined liquids. The nucleation mechanisms which initiate the solidification of the supercooled liquid are to date not entirely understood.

We present a comparative calorimetric study on different confined liquids (N_2, Ar, CO) which elucidates the decisive influence of grain boundaries and crystal structure of the solidified material on the freezing transition.

O 39.2 Tue 15:15 H42

Modelling laser-induced dielectric breakdown: Application of the multiple rate equation — •Oliver Brenk, Nikita Medvedev, and Baerbel Rethfeld — TU Kaiserslautern, 67663 Kaiserslautern, Deutschland

Material processing with ultrashort laser pulses is in the focus of experimental and theoretical research. In order to provide a tool for numerical simulation of the effects of ultrashort laserpulse irradiation on dielectrics the multiple rate equation (MRE) has been introduced [1]. The MRE allows to investigate the temporal evolution of the electronic density in the conduction band with very good agreement to a full kinetic approach [2], using Boltzman's equation, but with considerably less computational effort. We have extended the MRE model to include additional effects, namely the reflectivity and the recombination into Self-Trapped Excitons (STE-States). The reflectivity, depending on the electronic density, influences the laser intensity inside the material. STEs are localized electron-hole pairs formed by free electrons having recombined with localized holes, energetically lying between valence band and conduction band. Re-excitation out of these states is considered as well. We study the influence of these processes on the optical parameters and on the threshold behavior of dielectric breakdown. To further expand the model we plan to add a spatial dimension, to study the spatially resolved evolution of the electronic densities to the already implemented time evolution.

[1] B. Rethfeld, Phys. Rev. Lett., 92:187401, 2004.
[2] A. Kaiser et al., Phys. Rev. B, 61:11437, 2000.

O 39.3 Tue 15:30 H42

Influence of H_2O adsorption on the charge-density wave phase of 1T-$TiSe_2$ — •Matthias May, Stephan Thürmer, Cristoph Janowitz, and Recardo Manzke — Humboldt-Universität zu Berlin, Institut für Physik, Newtonstr. 15, 12489 Berlin, Germany

The transition-metal dichalcogenide $TiSe_2$ reveals a charge-density wave (CDW) phase transition at low temperatures and the driving force of this CDW is still under discussion (see e.g. [1]). One crucial question for the microscopic origin was that on the electric character, i.e. whether $TiSe_2$ is a semiconductor or a semimetal [1,2]. This has been answered by Rasch et al. [2] by means of angle-resolved photoemission (ARPES) and applying the effect of H_2O adsorption onto the van der Waals-like surface, bending the bands and resulting in a filled lowest conduction band. These ARPES experiments were continued at BESSY investigating now the influence of H_2O adsorption on the CDW transition at different temperatures. Results are discussed in context of the related theories.

[1] H. Cercellier, C. Monney, F. Clerc, C. Battaglia, L. Despont, M. G. Garnier, H. Beck, and P. Aebi, Phys. Rev. Letters 99, 146403 (2007)
[2] J. Rasch, T. Stemmler, B. Mueller, L. Dudy, and R. Manzke, Phys. Rev. Letters 101, 237602 (2008)

O 39.4 Tue 15:45 H42

New self-consistent model of ultrashort laser irradiation of materials — •Nikita Medvedev and Baerbel Rethfeld — Technical University of Kaiserslautern, Department of Physics, Erwin Schroedinger Str. 46, 67663 Kaiserslautern, Germany

We present a new model describing femtosecond laser interaction with a semiconductor or dielectric target. Based on the earlier developed Multiple Rate Equations [1], the model includes interaction of electrons with the phononic subsystem, allowing direct determination of conditions for crystal damage. Taking into account dynamical changes of the optical properties of the target (reflectivity, absorption coefficients), the developed model gives access to a criterion of the damage self-consistently, tracing a change of optical properties as well as a lattice heating and melting.

In contrast with commonly used approaches based on the thermodynamical description of the material (like two temperature model), our model is widely applicable for nonequilibrium electronic conditions, where one cannot use such thermodynamical property as temperature. On the other hand, the model is still simple to use. Applying experimental parameters, we found perfect agreement with the measured reflectivity of the material during irradiation with a femto-second laser pulse and also obtained the damage fluence threshold in very good agreement. The developed model is a powerful tool to describe the dynamics of the electronic subsystem as well as lattice heating.

[1] B. Rethfeld, Phys. Rev. Lett. 92, 187401 (2004)

O 39.5 Tue 16:00 H42

Lattice Gas Monte Carlo Simulations of Pentacene on Cu (110) - (2×1)O — •Johannes Gall, Michael Hohage, Chunyang Liu, Daniel Queteschiner, Günther Weidlinger, Lidong Sun, and Peter Zeppenfeld — Institute of Experimental Physics, Johannes Kepler University, Linz, Austria.

A reversible two-dimensional phase transition of pentacene (5A) submonolayer films on the Cu(110) - (2×1)O reconstructed surface has been observed. Several Monte Carlo (MC) and Kinetic Monte Carlo (KMC) simulations of a lattice gas Ising model have been performed to understand the behavior of the system. The combination of MC and KMC simulations allows investigating the role of kinetic processes during the phase transition. In the simulations different interaction models have been investigated. In particular, we find that the characteristics of the phase transitions strongly depend on the anisotropy of the lateral interactions. The simulation results are compared to recent RDS (reflectance difference spectroscopy) and STM (scanning tunneling microscopy) experiments.