DY 7: Modeling and Data Analysis

Time: Monday 10:00–11:45 Location: BH-N 128

DY 7.1 Mon 10:00 BH-N 128

MD simulations on martensitic transformations in iron-palladium — •Alexander Holm[1,2] and Stefan G. Mayr[1,2] — [1]Leibniz Institute of Surface Engineering (IOM), Leipzig — [2]Division of Surface Physics, Felix Bloch Institute for Solid State Physics, Faculty of Physics and Earth Sciences, University of Leipzig

We report about molecular dynamics (MD) simulation studies on martensitic transitions in iron-palladium (Fe_7Pd_3) shape memory alloys, mentioning custom-designed embedded atom method (EAM) potentials based on density functional theory (DFT) calculations. Upon application of an uniaxial compressive strain to the simulation cell it was found that the transformation from a face centered cubic crystal-lattice-configuration to a body centered tetragonal configuration occurs, exhibiting orientation variants which can be connected to the structural phenomenon of twinning, which is a prerequisite for the shape memory effect in Fe_7Pd_3.

The focus of this presentation will lie on the structural properties of the martensitic phase transition, regarding transformation paths and the introduction of a new method to determine structural changing incidents from a series of radial distribution functions, the *RDF-Separation-Function*.

DY 7.2 Mon 10:15 BH-N 128

Monte Carlo Simulations of Poly(3-hexylthiophene) aggregation — •Jonathan Gross and Wolfhard Janke — Institut für Theoretische Physik, Universität Leipzig,

Poly(3-hexylthiophene) (P3HT) is a semiconducting polymer that has applications in organic photovoltaics. It is widely used as a semiconducting layer in organic thin film field effect transistors (FETs) and solar cells. We found that a recently developed coarse-grained model [1] of P3HT, is suitable and able to reproduce not only fully atomistic simulations, but also experimental results [2, 3, 4]. On the basis of those single-chain studies, we now take the next step and look at aggregation of a few polymers, to gain an understanding of the fundamental processes that happen during the crystallization of P3HT. With replica-exchange (parallel tempering) simulations we investigate a system of a few short P3HT chains in the presence of a Au(001) surface and without a substrate.

[1] D. M. Huang, R. Faller, K. Do, and A. J. Moule, J. Chem. Theory Comput. 6 (2010) 526.

[2] S. Foerster, E. Kohl, M. Ivanov, J. Gross, W. Widdra, and W. Janke, J. Chem. Phys. 141 (2014) 164701.

[3] J. Gross, M. Ivanov, and W. Janke, J. Phys.: Conf. Ser. 750 (2016) 012009.

[4] M. Ivanov, J. Gross, and W. Janke, Eur. Phys. J. Special Topics 226 (2017) 667.

DY 7.3 Mon 10:30 BH-N 128

Temporal and spatial characteristics of electron cascades triggered by X-ray photons in LiF — •Vladimir Lipp[1], Nikita Medvedev[2], and Beata Ziaja[1,3] — [1]CFEL at DESY, Hamburg, Germany — [2]Institute of Physics and Institute of Plasma Physics, Academy of Science of Czech Republic, Prague, Czechia — [3]Institute of Nuclear Physics, Polish Academy of Sciences, Krakow, Poland

Low-fluence X-ray irradiation of alkali halides may cause long-living lattice defects called color centers. It is assumed that their spatial distribution reflects the X-ray beam shape and, therefore, may serve as an efficient diagnostic tool for the spatial pulse profile [1]. The color centers may be created via exciton decay mechanism; excitons are created when self-trapped valence holes catch free electrons, both produced by an intense X-ray pulse. However, X-ray-induced energetic photoelectrons trigger secondary electron cascades, which may strongly influence the final distribution of the valence holes before their self-trapping, and thereby of the color centers. Our in-house classical Monte-Carlo simulation tool XCascade-3D [2] follows the electron cascades in time and space. It provides distributions of the electrons and holes in various X-ray-irradiated materials, including alkali halides. For the study case of LiF, we present the corresponding calculations which enable to establish a connection between the experimentally measured distribution of the X-ray-induced color centers in LiF and the spatial shape of the X-ray beam – with potential experimental applications. References: [1] Pikuz, Faenov, Matsuoka et al., Scientific Reports 5, 17713 (2015). [2] Lipp, Medvedev, Ziaja, Proc. SPIE 10236, 102360H (2017).

DY 7.4 Mon 10:45 BH-N 128

Phase field modeling of diffusion-limited precipitation in multi-component Ni-based superalloys — •Markus Holzinger, Michael Fleck, and Uwe Glatzel — Metals and Alloys , University Bayreuth, Germany

We develop a phase-field model for the simulation of phase transformations in metallic multi-component alloys (Ni-based superalloys) with industry-relevant chemical complexity. This model is built to take into account thermodiffusion, elastic effects and inhomogeneities. The thermodynamic formulation is validated by comparisons to respective CALPHAD equilibrium calculations using the commercial program ThermoCalc. Furthermore, an elastic term is included in the model to account for the misfit stresses as well as elastic inhomogeneities between the two considered phases. We consider the coarsening kinetics of γ'-precipitates in single crystalline Ni-based cast-alloys. Here we show the results of a elastic strain simulation. We also discuss the results in comparison with experiments.

DY 7.5 Mon 11:00 BH-N 128

Breathing with the beating of the heart: A machine-learner's approach to ECG-derived respiratory signal estimation — •Stephan Bialonski[1], Daniel Vorberg[2], and Justus Schwabedal[3] — [1]Center for Advancing Electronics Dresden (cfaed), TU Dresden — [2]Max-Planck-Institute for the Physics of Complex Systems, Dresden — [3]Department of Biomedical Informatics, Emory University School of Medicine, Atlanta

We investigated how machine learning models can be used to extract knowledge from biophysical systems. As a test case, we studied the challenge to derive respiratory information from electrocardiographic (ECG) signals, a long-standing problem in sleep research. We identified two well-known coupling mechanisms by analyzing a long short-term memory (LSTM) architecture that we fitted to predict respiratory information from ECG signals. These mechanisms couple heart beat dynamics and respiration and comprise of a physiological coupling (respiratory sinus arrhythmia) as well as a physical coupling that is related to the position of measurement electrodes relative to the heart. We verified these results by modelling the coupling mechanisms and studying the resulting patterns in our LSTM architecture.

DY 7.6 Mon 11:15 BH-N 128

Profile likelihood based analyses of infectious disease models — •Christian Tönsing[1], Jens Timmer[1,2,3,4], and Clemens Kreutz[1,2,4] — [1]Institute of Physics, University of Freiburg, Freiburg im Breisgau, Germany — [2]Freiburg Center of Data Analysis and Modeling (FDM), University of Freiburg, Freiburg im Breisgau, Germany — [3]BIOSS Centre for Biological Signalling Studies, University of Freiburg, Freiburg im Breisgau, Germany — [4]Center for Biosystems Analysis (ZBSA), University of Freiburg, Freiburg im Breisgau, Germany

Ordinary differential equation (ODE) models are frequently applied to describe the dynamics of epidemics. In this work, we use such models of infectious diseases for the estimation of a priori unknown model parameters and their uncertainties from the information contained in recorded data of infected individuals. A deterministic multistart optimization approach is applied for parameter estimation. Moreover, we introduce profile likelihood-based uncertainty analyses and check the identifiability of a simple SIR model with data from an influenza outbreak at an English boarding school in 1978. Furthermore, a complex ODE model for vector-borne diseases with data from the Zika virus (ZIKV) outbreak in Colombia in 2015/16 is used for data-based model reduction utilizing likelihood profiles.

DY 7.7 Mon 11:30 BH-N 128

Modelling of non-Gaussian stochastic processes with memory — •Katja Polotzek and Holger Kantz — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Many real world phenomena such as wind speeds and rainfall amounts do not follow a Gaussian distribution. Among other shapes events might occur in an asymmetric or one-sidedly bounded manner. We obtain models for such situations by applying nonlinear transforma-

tions to Gaussian processes. By an appropriate choice of the transformation we can not only adjust the model distribution to the empirical data but also infer properties of the model from the well understood underlying Gaussian process. In particular, we are interested in the behaviour of the autocorrelation function and the memory structure of the stochastic processes. We illustrate the method by modelling daily rainfall amounts, which exhibit indications of long-range dependence.