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Editorial

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Materials have become an ever more important factor in most advanced technologies. It was no coincidence when the former State Secretary Christoph Matschie stated, at the opening of *WING* (Materials Innovations for Industry and Society initiated by the German Ministry for Education and Research), that nearly any new product is based on the improvement of an engineered material. This comes along with a constant quest for new materials, improved performance and decreased development costs. This quest is particularly strong for high-wage countries in the global market situation. Thus there is a steadily growing importance of systematic materials development supported by computer simulation methods in tailoring new materials for more and more specific demands for a wide range of applications from everyday household goods to opto-electronics and even further to medicine. In this context the tailoring of materials interfaces, respectively that of corresponding condensed matter systems, often used as model systems for the first ones, plays a particularly important role. The reason for this is that a material's functional properties are to a large extent determined by its inner and outer interfaces. Prominent examples are corrosion-resistant surfaces of household goods, or likewise inert surfaces of prostheses engineered for medical applications. During materials processing the inner and outer interfaces of such functional materials evolve driven by the complex interplay of all the physical and chemical mechanisms contributing to interface energetics, interface kinetics and interface dynamics. Essentially, this opens a multiscale problem ranging from the quantum mechanical to the continuum scale.

Indeed, materials science simulation methods have matured to this point. There has been a growing impact on materials development by modeling and simulation at all the relevant length scales (quantum-mechanical, atomic, mesoscopic, continuum) [1–3]. Dedicated methods have been designed for each length scale as well as methods to address scale-bridging phenomena (multiscale modeling [4]). The success of these methods can be seen in the fact that gradually the emphasis in materials modeling has shifted from explaining experimentally observed properties of materials to predicting not yet measured properties.

Such multiscale approaches, however, are by no means standardized, yet. They evolve with the demands pictured above. More precisely their development is an ongoing scientific field driven by the collaborative advances of chemists, physicists, mathematicians and computer scientists addressed by the engineers again and again with new specific problems of industrial impact with additional challenges for modeling and simulation. The first provide physically and chemically motivated model derivations, which need to be programmed as efficiently as possible. For the latter, advanced numerical schemes developed in the related mathematical and computer science departments play a crucial role. Moreover, such models need to be verified by comparison to experiments or to other model approaches or even to specific limits, in which they can be analyzed based on tools from analytical mathematics. The latter

analytical mathematics also provides additional methods for model derivation, which can be combined with the already mentioned approaches from physics and chemistry to develop enhanced models.

This volume focuses on recent advances in the computational design of condensed matter interfaces, which have been obtained lately based on the above multidisciplinary approach. To that end it takes a tour through contributions of Computational Materials Engineering with selected topics as diverse as glass corrosion, epitaxy, solidification of classically structured materials and contributions to materials of the biomedical area. The contributions start with an analytical focus on the derivation of suitable modeling approaches, continue with achievements in modeling material properties, and finally set the focus on numerical improvements to cope with the ever-increasing computational effort.

In particular, recent advances in the rigorous derivation and evaluation of two-scale models for liquid–solid interfaces provide a computationally efficient simulation technique that couples surface structure formation on the discrete particle scale to continuum equations for embedding fluid flow such that the numerical grid for continuum modeling is independent of the scale of the microstructure. Eck and Emmerich employ this development as a prerequisite for the further extension of the model by elastic interactions at the interface, which allows for the simulation of liquid phase epitaxy of strained films on a substrate of different lattice parameter. Kundin et al. generalize the two-scale model to stepped surfaces with varying adatom diffusivities and arbitrary diffusion barriers at step edges (Ehrlich–Schwoebel barriers). Both contributions demonstrate step by step how standard model expressions such as the Navier–Stokes equations or the Gibbs–Thomson relation are suitably reformulated on both involved scales and how a systematic testing of the model performance and errors can be achieved by analyzing exactly tractable limiting cases. As such considerations are at the very beginning of any systematically sound derivation of multiscale approaches, a high level of detail is chosen for didactic reasons. Both contributions focus on solid–liquid interfaces, which involve strong local changes of order parameters, and hence are very demanding. Such models may be adjusted to the large-scale classical simulation of other interface types such as liquid–liquid or solid–solid, and the present issue aims at stimulating research in those directions.

Parameters for such large-scale modeling of interfaces may have to be derived from simulations on a smaller scale, because material properties in the vicinity of an interface differ from experimentally accessible bulk properties due to the presence of interface-induced gradients of the elastic tensor tractable by finite-element modeling, the chemical potential in a grand-canonical formulation or the mean inner electrostatic potential in a quantum-mechanical formulation. Three contributions provide insight into the implementation of this strategy starting from first-principles data for selected topics from interface modeling. The tutorial review by Lymperakis et al. introduces first-principles and atomistic potential techniques as well as the basic classification of solid–solid interfaces. The authors demonstrate how modern empirical potentials reliably reproduce first-principles results on grain boundary structure and energetics and how they can be employed to extend first-principles data to more complex structures, including the link to classical particle density functional theory for the liquid–solid interface. The coupling of quantum-mechanical and classical force-field simulations is described in more detail in the contribution by Knaup et al. for examples of an imidazole-based polyelectrolyte fuel cell layer and for an epoxy-based adhesive film on aluminum oxide. The study focuses on interface reactivity, sets criteria for the selection of either hierarchical or concurrent coupling and demonstrates how the required size of the quantum-mechanically treated core is systematically evaluated for the latter case. Likewise, electronic transport is strongly influenced by interfaces between different components of an electronic device, where materials with different bonding and conductivity properties are joined and the local electronic structure at the interface again differs from those in the pure bulk phases. Methods to simulate ballistic, defect-induced, hopping and phonon-assisted shuttling transport of carriers from the quantum-mechanical to the continuum range are revisited in the overview by Gemming et al., with specific focus on the influence of interfaces on the derivation of parameters for large-scale modeling from first-principles data. Beyond the topics covered here, namely stability, reactivity and conductivity, there exist many more exciting phenomena at and across interfaces, for instance with regard to magnetic, optical, ferroelectric

or multiferroic properties, and future efforts in these fields will have to rely on similar multiscale approaches.

The efficient simulation of thermodynamic properties and phenomena by combined particle-based and continuum approaches is at the heart of four further contributions, which aim at assessing the influence of temperature, composition and long-range interactions. Schrader et al. present methods of extracting interfacial free energies of flat and curved interfaces at liquid–vapor and liquid–solid interfaces to study the evolution of the interface close to a coexistence point. The study focuses on the derivation of surface free energy expressions for simple model systems from statistical mechanics such as the Ising lattice-gas and Lennard-Jones and hard-sphere fluids in order to lay the grounds for a similar derivation for more complex statistical models. In this way, both the basic steps become transparent and reference data are provided, which may serve as a limiting case for the evaluation of more complex models. Polyelectrolyte layers, i.e. regular multilayered structures composed of alternating layers of polycations and polyanions, are a particularly intricate material, because long-range interactions are triggered by rather short-range atom or functional group dynamics. Cerdà et al. compare a mesoscopic large-scale bead–spring model with Langevin dynamics and fully atomistic molecular dynamics for the structure evolution of the first deposition layer under wetting or dewetting conditions and derive criteria for the enhancement of the mesoscopic approach based on the results of the atomistic simulations. In contrast, a concurrent coupling scheme between a particle-based coarse-grained model for a binary polymer blend and continuum description in terms of a time-dependent Ginzburg–Landau approach for the evolution of the order parameter within such a binary system is presented by Müller. The inherent divide-and-conquer strategy allows the efficient computation of composition fluctuations up to the spinodal decomposition regime. Spinodal decomposition is also the topic of a contribution by Lecoq et al., who extended the Cahn–Hilliard equation to include memory effects by a hyperbolic term. Large-scale simulation and careful comparison with the standard Cahn–Hilliard formulation show that, in particular, the short-time dynamics of the phase transition is affected. The present contributions go beyond a standard treatment of interface dynamics and highlight the non-equilibrium thermodynamic conditions that lead to interface creation.

Aspects concerning numerical implementation have only briefly been addressed in the studies described so far. The final two contributions focus on particular details concerning computational materials modeling of dislocation and solidification dynamics in materials with high application relevance in engineering. Dislocation motion is a key ingredient for understanding material strength during plastic deformation, as both desired dislocation hardening and unfavorable dislocation-based failure phenomena are based on the same atomistic processes. Owing to granular formulation of the model equations by Beneš et al., the present parametric simulation method for dislocation dynamics is a parallelized, computationally efficient approach to study the interplay between mobile and sessile defects. An adaptive discretization of the line shape by short straight segments allows the simulation of extended glide dislocations and localized loops with equal accuracy. Finally, Siquieri et al. report on the two-scale modeling of dendritic growth, which is obtained during solidification in convective iron–manganese alloys under an externally forced flow field. A detailed description of the simulation setup and the discretization of phase-field equations on a numerical grid is followed by a quantitative evaluation of the differences between structures formed with and without the forced flow field. Both contributions address the physics underlying typical engineering processes such as plastic deformation and dip-coating or casting. By comparison with experimentally observed structures, they allow one to rationalize which microscopic mechanism is the decisive one under a given set of external conditions and open a perspective for the modeling of ever more complex processing steps from engineering.

In conclusion, all examples addressed in the present contributions highlight different aspects of the methodological further development in the computational field necessary to support their design. These involve recent issues of the required mathematical analysis, model development and advanced numerics and thereby demonstrate how their synergetic combination contributes essentially to advances of the field. We hope that this multidisciplinary overview can constitute a still missing reference material that creates awareness for contributions from the “other sides”

to each of the specific scientific communities involved, in particular where they start to overlap. Thereby we hope to provide an additional cornerstone to push this demanding, and at the same time rapidly evolving, field.

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