To predict the failure and strength properties of metallic alloys, it is neccessary to take in account the behaviour of such material under the influence of elastic forces. When applying a sufficient amount of stress, the grain structure breaks and forms a crack. In numerical simulations, we investigate crack propagation in polycrystalline metallic alloys for mode I and III. The shape of such cracks depends on the applied loads and on the grain distribution of the observed material. Suitable simulations require many grains in a relatively large domain. To achieve this goal, we present a parallel, optimized multi phase field model featuring efficient modelling of large three dimensional phase systems coupled with a model for elastic stresses. We show results for 2D and 3D crack developments along grain boundaries and in polycrystalline systems.

MM 20.16 Tue 14:45 P4

From DFT to TB: A reliable derivation of tight-binding parameters for hard materials — •Martin Reese[1,2], Matous Mrovec[1,2], Bernd Meyer[3], and Christian Elsässer[2] — [1]IZBS, Universität Karlsruhe — [2]Fraunhofer-Institut für Werkstoffmechanik IWM, Freiburg — [3]ICMM, Universität Erlangen-Nürnberg

Hard materials play an important role in industrial applications as protective coatings of tools. Recent experiments indicate that nanostructered composites of crystalline and amorphous carbides and nitrides can yield materials that reach the limit of super-hardness. However, a scientific understanding of these complex materials is still incomplete.

In the course of developing a multi-scale modelling framework for simulations of nanocrystalline transition metal carbides and nitrides we apply accurate first-principles calculations, based on the density functional theory (DFT), to derive reliable non-orthogonal and orthogonal tight-binding (TB) Hamiltonians. The TB Hamiltonians are constructed by projecting the self-consistent electronic wave functions from DFT onto a minimum basis set of atomic orbitals. This well defined procedure enables to overcome the ad-hoc fitting of TB models and presents a rigorous coarse-graining tool, which can be applied in various bonding environments. In this contribution we will present the application of the method to several model materials, namely the covalently bonded elements carbon and silicon, the transition metal titanium, and binary compounds of these elements. We will discuss the variation of the Hamiltonian matrix elements as a function of the interatomic distance and their transferability in various environments.

MM 20.17 Tue 14:45 P4

Modelling particulate self-healing materials and application to uni-axial compression — •Olaf Herbst[1,2], Akke Suiker[1], and Stefan Luding[2] — [1]Aerospace Engineering, TU Delft, Kluyverweg 1, 2629 HS Delft, The Netherlands — [2]2Multi Scale Mechanics, TS, CTW, UTwente, P.O. Box 217, 7500 AE Enschede, The Netherlands

Using an advanced history dependent contact model for DEM simulations, including elasto-plasticity, viscosity, adhesion, and friction, pressure-sintered tablets are formed from primary particles. These tablets are subjected to uni-axial compression until and beyond failure displaying peak strength. For fast and slow deformation we observe ductile-like and brittle softening, respectively.

We propose a model for local self-healing that allows damage to heal during the loading process such that the material strength of the sample increases and failure/softening is delayed to larger strain. Local healing is achieved by increasing the (attractive) contact adhesion forces for those particles involved in a potentially breaking contact.

We examine the dependence of the strength of the material on (a) the damage detection sensitivity, (b) the damage detection rate, and (c) the (increased) adhesion between healed contacts. The material strength is enhanced, i.e. the material fails at larger strains and reaches larger maximal stress values, when any of the parameters (a) – (c) is increased.

MM 20.18 Tue 14:45 P4

The relationship between the sinter-atmosphere and the phase modification of TiO_2 at high temperatures — •Nicole Pfeiffer, Abdelilah Lahmar, Salah Habouti, Matthias Dietze, Claus-Henning Solterbeck, and Mohammed Es-Souni — Institute for Materials and Surface Technology, University of Applied Sciences Kiel, Germany

In this work we generated TiO_2-nano particles on Si-substrate by solution deposition from a precursor. The films were treated under different atmospheres at ∼800°C to control the phase formation. It is shown by means of Raman scattering that anatase polymorph forms preferentially in reducing atmosphere, instead of the thermodynamically stable rutile phase. The results are discussed in terms of specific defect structures that could form in the anatase phase.

MM 20.19 Tue 14:45 P4

Performance analysis of a parallel simulator for phase-field models — •Alexander Vondrous, Michael Selzer, Britta Nestler, and Marcus Jainta — Institute of Computational Engineering (ICE), Karlsruhe, Germany

Parallel algorithms for the numerical solution of phase field models are used to improve calculation times. To simulate a large section of a complex microstructure and to consider effects such as fluid flow on the morphology evolution, large computational domains have to be considered. In such cases parallelization is needed to significantly increase the speed of the computation. To classify the performance of parallel computations, infomation about the used hardware is important. Performance characteristics are, among others, the speedup and the efficiency. The results of the presented performance analysis are used to optimize parallel algorithms and hardware utilization. The numerical scheme avoids calculations in bulk phase regions of the domain leading to an inhomogeneous load balance and an undesirable higher idle time of some of the CPUs in the network. To minimize this effect, dynamic domain decomposition during run time is applied. Simulations of dendritic growth in a flow field serve to evaluate the performance for different numbers of CPUs.

MM 20.20 Tue 14:45 P4

Polarization dependent Raman spectroscopy of $LiBH_4$ single crystals — •Britta Willenberg, Florian Gebert, and Joachim Schoenes — Institut für Physik der Kondensierten Materie, TU Braunschweig, 38106 Braunschweig, Germany

In a previous paper [1] we have reported an extensive low temperature Raman scattering study on $LiBH_4$ and $LiBD_4$ powders. The 27 observed lines have been assigned to phonon modes within the orthorhombic Pnma structure by comparing the experimental values to density functional theory (DFT) values [1]. In the present contribution we present for the first time Raman scattering measurements on small $LiBH_4$ single crystals. These have been identified among the grains of the powders (Alpha Aesar) by searching for large polarization dependencies of the Raman lines. On the basis of these new results a few of the former assignments have to be revised. Among the external modes this concerns the mode near 307 cm^{-1} which is definitely of A_g symmetry and not of B_{2g} symmetry as had been concluded on purely energy arguments.

A second issue is the phase transition to a hexagonal structure at about 380 K. Several grains of our powder samples did not show the anticipated changes of the Raman spectra. We have now succeeded in finding a few grains which, indeed, display the characteristic simplification of the Raman spectra when the phase transition to the hexagonal phase occurs.

[1] A.-M. Racu et al., J. Phys. Chem. A 112, 9716 (2008)

MM 20.21 Tue 14:45 P4

Low temperature Raman spectroscopy of $Mg(BH_4)_2$ and $Mg(BD_4)_2$ — •Florian Gebert[1], Britta Willenberg[1], Joachim Schoenes[1], Michiel van Setten[2], Christoph Frommen[2], and Maximilian Fichtner[2] — [1]Institut für Physik der Kondensierten Materie, TU Braunschweig, Germany — [2]Institute of Nanotechnology, Forschungszentrum Karlsruhe, Germany

We report a micro-Raman scattering study on fine powders of $Mg(BH_4)_2$ and $Mg(BD_4)_2$ for temperatures ranging from approximately 5K to room temperature. At the lowest temperature, we observe 25 lines in both compounds, which were assigned within the 86 Raman active modes, for the I-4m2 structure, whose energies have been derived using first principle calculations based on density functional theory. This structure was claimed by Ozolins et al. [1] to posses an even lower ground state energy than the $P6_1$ structure reported formerly for the low temperature α-phase [2,3]. The comparison of theoretical and experimental values leads to straight lines with slopes between 0.98 and 1.03 for the external, bending and stretching modes, which is better than expected. Nevertheless, one can not definitively conclude that the structure is I-4m2 since a substantial number of possible lines have not been observed. This is even more so for the $P6_1$ structure. Further progress will require measurements on single crystals and/or intensity computations. [1] V. Ozolins et al., Phys. Rev. Lett. 100, 135501 (2008) [2] R. Cerný et al., Angew. Chem. Int. Ed. 46, 5765 (2007) [3] J.-H. Her et al. , J. Acta Cryst. B63, 561 (2007)