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Multiscale Simulations of Metals

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Summary

The aim of this project is to develop methods and algorithms for connecting an elastic-plastic continuum, which is modelled with Finite Elements (*FE*) and Dislocation Dynamics (*DD*) by parameters (vertical method - in contrast to a horizontal method where scales are connected within one model) to an atomistic system dealt with Molecular Dynamics (*MD*) or Monte Carlo (*MC*) simulations (Figure 1). Combining of methods is relevant in the frame of multiscale hybrid continuum-atomistic simulations of precipitation strengthened materials such as steels or lightweight metals, where macroscopic mechanical properties, like crack initiation and crack propagation energies, depend on precipitation sizes as dislocation-particle interaction energies in metals are particle size dependent. Due to the strongly different length scales, the parameters responsible for the mechanical behaviour of the particle strengthened metals are different for the atomic level, for the mesoscopic dislocation level as well as for the micromechanical and atomistic length scales. On the finite element level, the sensitive parameters for deformation and fracture are typically related to stress-strain-curves as well as to macroscopic yield and fracture strengths from experiments. On this macroscopic level,

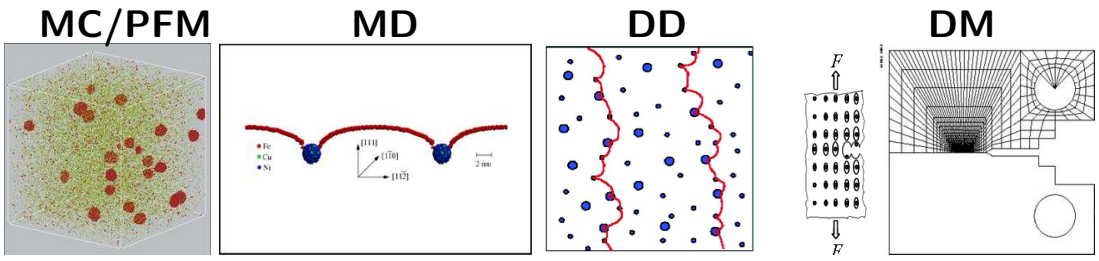

Figure 1: Simulation of the coarsening of the microstructure by Monte Carlo (MC) and Phase Field Methods (PFM); dislocation-particle interactions are simulated by Molecular Dynamics (MD) as well as Dislocation Dynamics (DD) methods; material failure is simulated in the framework of damage mechanics (DM). The following **coupling parameters** will be derived in this **vertical simulation**: particle size distributions (MC for small particle sizes and PFM for larger ones), interface energies (MD) and strengthening levels (DD, MD).

the size distributions of the precipitates are indirectly included within the macroscopic stress-strain curve. On the *DD* continuum level the particles can be taken into account explicitly for a wide variety of sizes. Distributions of particles and the interaction of dislocations with a field of particles could provide realistic yield strengths and fracture strengths of these composites as input parameters for the macroscopically required stress-strain curves. *DD* simulations frequently lack from interaction energies between dislocations and discrete particles. The derivation of such parameters requires a smaller or, more precisely, an atomistic length scale to be introduced as e.g. by *MD* computer simulations where dislocation line energies can be derived for geometric situations which appear during the interaction between a dislocation and the particles. On all length scales, temperature dependent material properties are required such as stress-strain curves, dislocation line energies as well as the vibrations of the atoms. Finally, the required particle size distributions, as they are present after material production or from tempering or annealing procedures, can be derived from *MC* simulations where diffusion processes are responsible for the particle size increase (Ostwald ripening) which is empirically described within the Lifshitz-Slyozow-Wagner (*LSW*) theory. A second possibility, to derive the laws especially for larger precipitates is to apply phase field methods (*PFM*) to simulate the particle coarsening process. A physically founded description of the growth of the particles is highly needed as input for the simulation of particle growth after nucleation as well as for deriving *PFM* energy parameters, such as interface energies or dislocation line energies. The underlying backgrounds for the *MC* approach are physical ground states of the atoms, attempt frequencies and local binding energies based on theory and experiments.

There are numerous approaches to solve this problem, like direct coupling procedures within one algorithm (horizontal connection) - with the difficulty of highly divergent length and time scales to be connected. A promising proposal derived in the recent past covers on each length scale the relevant problem with the appropriate method and bridges the gaps by handshakes through parameter transfer (hierarchical or sequential modelling). Preliminary work has been done in the past by bridging length and time scales directly (horizontal connection) within a coupled Finite Element Atomistic (*FEAt*) approach for part of the problem or by hierarchical simulations with several required simulation tools. As a first step, the available direct coupling procedures have to be carefully checked for possible modifications in order to develop these methods further. As a practically relevant application of such an approach, precipitation strengthening of steel or of an Al-alloy shall be tackled in this work and be compared with experiments. Parametric studies will provide an overview of the possibilities in materials to be further developed.

Experience has been gained in our own group in continuum and atomistic simulations with *FE*, *MD*, *MC* as well as in *PFM* methods and damage mechanics (*DM*). For the *FE* and *MD* simulations we will closely cooperate with *SimTech* researchers and with groups from *Research Area B* which are well experienced in continuum and atomistic methods and which are also concerned with direct coupling approaches.

Especially, it is the aim of the coupling between dislocation dynamics (*DD*) and damage mechanical (*DM*) crack propagation simulations to derive the strength increase for realistic distributions of precipitate sizes and arrangements as well as for particle densities obtained from Monte Carlo (*MC*) simulations and from phase field methods (*PFM*), respectively. *DD* is based on realistic simulation parameters from *MD* results for the complex interaction between a dislocation and a Cu-precipitate. The interaction between a dislocation and a particle can be simulated by *MD* as a function of the particle size. The increase of the strength level will be derived for realistic particle size distributions. This will be valuable for estimating the macroscopic strengthening effect due to the Cu-precipitates and consequently for deriving the failure behaviour of the material using *DM* in the frame of the finite element method (*FEM*).

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