6th European Conference on Computational Mechanics (ECCM 6)
7th European Conference on Computational Fluid Dynamics (ECFD 7)
11 15 June 2018, Glasgow, UK

# MULTISCALE SIMULATION OF PHASE CHANGE

**T. Willerding*[1] and M. Bischoff[2]**

[1] Institute for structural mechanics, University of Stuttgart, 70569 Stuttgart, Germany, willerding@ibb.uni.stuttgart.de
[2] Institute for structural mechanics, University of Stuttgart, 70569 Stuttgart, Germany, bischoff@ibb.uni-stuttgart.de

**Key words:** *Multiscale Simulation, Phase Change, Finite Elements, Molecular Dynamics*

Behavior of many materials shows effects that cannot be modeled on the macroscopic scale. These effects require micro-scale modeling and often quite different computational methods compared to those on the macro scale are used for this purpose (e. g. discrete methods instead of continuous methods). Particularly for design of new materials, for which the lack of experimental data excludes development of purely phenomenological material laws, predictive modeling of effects on the micro-scale may be crucial. Therefore it is attractive to combine different computational models within one framework. This is the goal of multi-scale modeling of materials.

Many methods have been developed in the past to bridge the huge gap between atomistics or molecular dynamics and classic continuum mechanics (see e.g. the book by Tadmor and Miller[2]). One important challenge is the modelling of atomistic effects at non-zero temperatures. The subject of the present study is a concurrent multi- scale strategy based on similar ideas as the FE2 approach. The method consists of combining the FE2 concept and molecular dynamics, making it more like FExMD.

Instead of resolving the problem completely with atoms, only a number of small molecular dynamics sub-problems are solved at each Gauss point. The kinematics of the coarse scale is applied to the molecular dynamics sub-problem (e. g. via the deformation gradient), which returns the constitutive behavior (e. g. in terms of resulting stresses). When using the right potential, e.g. the EAM potential by Meyer and Entel [1], phase change in iron between body-centered cubic and face-centered cubic can be simulated in a multiscale environment.

This approach has been implemented into the object oriented, modular finite element code NumPro, developed at the institute. A number of mechanical and thermal test cases have been calculated and the results are presented.

## References

[1] R. Meyer and P. Entel. “Martensite-austenite transition and phonon dispersion curves of $Fe_{1-x}Ni_x$ studied by molecular-dynamics simulations”. In: *Physical Review B* 57 (1998), pp. 5140–5147.
[2] E.B. Tadmor and R.E. Miller. *Modeling Materials: Continuum, Atomistic and Multiscale Techniques*. Cambridge: Cambridge University Press, 2011.