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MULTISCALE SIMULATION OF PHASE CHANGE

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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.

32, 1340, 2011. Multiscale Simulation of Phase Change Memory (PCM) Manjeri P. Anantram, University of Washington, DMR 1006182 To investigate energy efficiency during scaling, finite element method (FEM) has been used to analyze Ge 2 Sb 2 Te 5 (abbr. GST; most widely- used phase change material for PCM devices) model shown above. It is shown that more than 90% of the operation energy is wasted in the current PCM design. This ratio will largely remain the same if the device is scaled by k (k>1) times (left figure). Our results indicate that the energy efficiency of PCM devices can be significant Key words: Multiscale Simulation, Phase Change, Finite Elements, Molecular Dynamics. Behavior of many materials shows eects that cannot be modeled on the macroscopic scale. These eects require micro-scale modeling and often quite dierent computational methods compared to those on the macro scale are used for this purpose (e. g. discrete methods in-stead 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 eects on the micro-scale may be crucial. Therefore i This study implements a multiscale numerical simulation framework using finite element analysis to evaluate the influence of Phase Change Materials (PCMs) on the thermal response of concrete pavements in places with significant winter weather conditions such as New England area of the United States. The influence of transition temperature of PCMs, PCM-dosage, environmental and weather conditions are considered in the analysis. The analysis is carried out at different mutually-interactive length scales and the latent-heat associated with different PCMs is efficiently incorporated into the simul... A phase transition is self-consistently simulated on three different time-space levels. On the first level, we use ab initio quantum molecular dynamics calculations with taking into account temperature distribution. On the second level, time dependent evolution of the electronic density is simulated on basis of reduced Ehrenfest molecular dynamics near the line of the phase transition of the second kind. On the third level, we use a heat conduction equation in continuous media to calculate new temperature distribution.Â Popov A.M., Nikishin N.G., Shumkin G.N., (2014), MULTISCALE QUANTUM SIMULATION OF STRUCTURE PHASE CHANGE AND THERMAL DISRUPTION IN NANODOT OF AMORPHOUS CARBON. Computational nanotechnology, 1: 17-25. Reference list A multiscale computational method couple dual reciprocity boundary element method (DRBEM) with finite volume method (FVM) is developed, and used to numerically simulate the hydrothermal gasification and evaporation of micrometer scale particles in two-phase flow. The engineering applied background of the problems include: hydrogen production from biomass in supercritical water, water mist fire suppression, etc. Numerical results shows the multiscale computational method coupled DRBEM with FDM is credible and effective. This paper also presents some valuable numerical results for these engineer