A combined hierarchic-partitioned-domain method for phase change in metals

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ABSTRACT

Phase change between different lattice structures plays an important role in the formation of metals, e.g. iron or titanium. It is therefore of interest to simulate phase change in a multiscale context. As phase change requires an internal restructuring of the molecular layout, traditional multiscale methods cannot be used, as these require fixed coupling at the interface between coarse scale and fine scale and very often also in the coarse scale due to using the Cauchy-Born rule.

In order to overcome these limitations, a combined hierarchic-partitioned-domain method is proposed that consists of two parts. On the finite element (continuum) level, a method based on the FE^2-approach by Feyel [1] is used with molecular dynamics simulations as sub-problems, one sub-problem at each Gauss integration point. With molecular dynamics as material law for the finite elements, the finite elements behave in the same way as atoms for coarse scale deformations. Using this method, phase change can already be simulated in the coarse scale as small molecular dynamics sub-problems are sufficient for phase change simulation. This is the *hierarchic* part of the method.

The *partitioned-domain* part of the method consists of dividing the domain in two parts: a molecular dynamics and a finite element part. The coupling of finite elements and molecular dynamics at the interface is done with a new concept, where the coupling atoms are put into a box with periodic boundary conditions. The box has the shape of a parallelepiped and is deformed according to the finite element deformation. A close-fit parallelepiped approximation of this deformation is calculated from the node positions. The force on the bound atoms are redirected to the finite element nodes using shape functions of the finite elements in a slightly modified way to ensure that the forces are only enacting on the finite element faces that are on the interface side to the finite elements. The coupling with the periodic boundary condition box provides the coupling atoms with more freedom and enables them to change phase.

The method is validated in a number of test cases for the phase transitions between body-centered cubic and face-centered cubic lattice structure in iron and between hexagonal close-packed and body-centered cubic lattice structure in titanium.

REFERENCES

[1] Feyel, F. (2003). A multilevel finite element method (fe2) to describe the response of highly non-linear structures using generalized continua. Computer Methods in Applied Mechanics and Engineering, 192(28):3233 – 3244. Multiscale Computational Mechanics for Materials and Structures.