Efficient crystal defect simulations through atomistic/continuum coupling using boundary element techniques

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ABSTRACT

Computational material science is moving rapidly towards a quantitatively predictive field. This has been accomplished over the past three decades, thanks to the success of atomic-scale simulations involving multi-defect interactions and recent developments of very accurate and flexible machine learning potentials which can be directly calibrated to quantum mechanics [1]. This in turn, however, has led to the necessity of using massive supercomputers which becomes quickly uneconomic for larger problem sizes of the order several hundreds of nanometers.

This eventually brings back the need for efficient multiscale methods which restrict atomic resolution to parts of the domain where it is essential (i.e. in the vicinity of lattice defects) and employ linearized models in parts which undergo close to homogeneous deformation. In [2] we have developed such a coupled method where an infinite domain is split into a fully atomistic problem and a linear elasticity region, which we have solved using an exterior discrete boundary element method (DBEM). The high efficiency compared with classical fixed boundary conditions has been demonstrated for various test cases.

Here, we show some recent developments of this method, in particular, an extension to finite problems which allows the definition of complex boundary conditions. An efficient staggered solver is presented which is inspired by the theory of domain decomposition for partial differential equations and can be parallelized conveniently. If time permits we present an application of our three dimensional coupled atomistic/discrete dislocations method [3], where the complementary elasticity problem can now be solved efficiently with the atomistic/DBEM coupling.

REFERENCES

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