Atomistic submodel implementation and application within microstructure analysis by molecular dynamics

Ivan Trapić [1]*, Robert Pezer [2] and Jurica Sorić [1]

[1] University of Zagreb, Faculty of Mechanical Engineering and Naval Architecture,
Ivana Lučića 5, 10000 Zagreb, Croatia
e-mail: ivan.trapic@fsb.hr, jurica.soric@fsb.hr web page: www.fsb.unizg.hr/lnm/staff/

[2] University of Zagreb, Faculty of Metallurgy, Aleja narodnih heroja 3, 44103 Sisak, Croatia
e-mail: rpezer@simet.hr, web page: www.simet.unizg.hr/hr/o-fakultetu/Members/rpezer

ABSTRACT

Classical continuum mechanics faces substantial difficulties for adequately taking into account stress and strain distributions around microstructural material discontinuities [1] such as crystallographic defects, voids, and grain boundaries. One way to improve the microstructural model is the development of the atomistic submodel that provides a significant reduction of vast amounts of atomistic data and degrees of freedom in the areas without discontinuities.

In the proposed approach continuum model, discretized by finite elements, runs the atomistic submodel by providing boundary displacement field for atoms on the edge of the simulation cell [2] driven by molecular dynamics. Therefore, atomistic submodel is placed only around the areas where continuum models about to fail. Significant problem visible in such a composite model is the correspondence of the continuum and atomistic quantities like stress [3], strain and displacement.

First, we present a simple pedagogical 1D example of atomistic chain with Lennard-Jones interatomic potential that stresses the differences between atomistic and continuum models. Besides, we examine possible problems that might be faced connecting the two approaches. After that, the method is applied to the 2D example of graphene honeycomb lattice with AIREBO interatomic potential [4].

The presented procedure shows how one can use atomistic simulations in regions where the continuum mechanics model is about to fail or have to be formulated in a very complicated way. The final contribution is the utilization of the best from both worlds, speed of the continuum mechanics using finite elements methods and informing it by relevant material properties inferred from atomistic simulations by judiciously using molecular dynamics where it is the optimal choice.

REFERENCES

[1] I. Trapić, R. Pezer, J. Sorić, Atomistic Modelling of 2D Stress Distribution Around Discontinuities, Transactions of FAMENA (1333-1124) 42, 3; 47-60, 2018,

[2] S. Li, S. Urata, An atomistic-to-continuum molecular dynamics: Theory, algorithm, and applications, Computer Methods in Applied Mechanics and Engineering, Volume 306, Pages 452-478, 2016,

[3] N. C. Admal, E. B. Tadmor, The non-uniqueness of the atomistic stress tensor and its relationship to the generalized Beltrami representation, Journal of the Mechanics and Physics of Solids, 93, 72-92, 2016,

[4] D. W. Brenner, O. A. Shenderova, J. A. Harrison, S. J. Stuart, B. Ni, S. B. Sinnott: A second-generation reactive empirical bond order (REBO) potential energy expression for hydrocarbons, J. Phys.: Condens. Matter 14, P. 783–802, 2002