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Molecular dynamics simulation of stress distribution in 2D systems

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The need to produce down to atomistic scale accurate representations of mechanical deformation processes has been ever more and more important to power up new solutions to tackle modern technology challenges. Standard elastic theories within continuum mechanics approach provide a well-established framework to do practical engineering simulations at the macro scale with wide range of applications. One of the most promising techniques to scale resolution down to the nanolevel is molecular dynamics simulations (MDS). In this work stress distribution around circular opening has been analyzed in the atomistic model of single layer 2D atomistic system, with atom interactions described by realistic interaction potential. Calculations were conducted on the problem of stress distribution around the elliptic hole in 2D sheet subject to uniaxial loading. Results for atomistic stress, calculated as spatial average by using Hardy formulation. One of the goals in this research is development of the efficient switching adaptive mechanism for local continuum to atomistic simulation transition. Quantitative measure for local switching suitable for fast calculation in multiscale simulation is proposed. As an example we provide calculation results in graphene where we have plenty of benchmark data. We point out routes to the development of the fully physically driven strategy for continuum to atomistic coupling where computationally expensive MDS is triggered upon local conditions identification. MDS is run up to the fracture of graphene with investigation of the structural changes in relation to the various conditions like temperature and loading rate.

Keywords: molecular dynamics (MD), stress distribution, materials length scales

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