

Title of Paper:

Study of cluster based energy sampling quasi continuum method and its application to nano indentation

Authors:

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Abstract:

Atomistic to continuum scale bridging is a highly demanded research area. There are many quasi continuum methods developed which are briefly explained and compared in [1]. The accuracy and efficiency of the quasi continuum methods is a crucial criterion in comparison with the fully atomistic method. The concurrent multi scale method namely cluster based quasi continuum method proposed in [2] differs from the rest of methods. It provides atomistic coarse graining which prevents the atomistic to continuum interface complexity and thus gives seamless scale transition of crystalline solids at 0 K. The adaptive refinement strategy enforces fully atomistic resolution in the crystal if it require. The accuracy, efficiency and limitation of this method is assessed and critically evaluated.

The main focus of the contribution is to study the cluster based energy sampling quasi continuum method presented in [3] with application to nanoindentation in 3 dimensional space. The adaptive refinement strategy has been successfully employed which provides perfect atomistic resolution in the area where dislocations are present during plastic deformation. An outcome of this study, the method can be now effectively apply to the nanoindentation simulation at 0 K using embedded-atom method potential. The dislocation analysis of face centered cubic material like aluminum, copper, silver and body centered cubic material like iron, tungsten have been carried out by nanoindentation simulation in $\langle 0 0 1 \rangle$.

References:

- [1] Miller R.E., Tadmor E.B: Modelling Simul. Mater. Sci. Eng. 17:053001, 2009.
- [2] Knap J., Ortiz M.: J. Mech. Phys. Solids 49 (2001) 1899 – 1923.
- [3] Eidel B., Stukowski A.: J. Mech. Phys. Solids 57 (2009) 87-108.

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Topic:

A Mechanical Properties: Plastic Deformation, Fatigue, Fracture,