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Energy and force transition between atoms and continuum in quasicontinuum method

Shu-Wei Chang[1], Ying-Pao Liao[1], Chang-Wei Huang[2] and Chuin-Shan Chen[*1]

[1]*Department of Civil Engineering, National Taiwan University, Taiwan*
[2]*Department of Civil Engineering, Chung-Yuan Christian University, Taiwan*

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Abstract. We present a full energy and force formulation of the quasicontinuum method with non-local and local transition elements. Non-local transition elements are developed to transmit inhomogeneity from the atomistic to the continuum regions. Local transition elements are developed to resolve the mathematical mismatch between non-local atoms and the local continuum. The rationale behind these transition elements is provided by analyzing the energy and force transitions between atoms and continuum under the Cauchy-Born rule. We show that breakdown of the Cauchy-Born rule occurs for slaved atoms of local elements within the cutoff of non-local atoms. The inadequacy of the Cauchy-Born rule at the transition region naturally leads to the need of atomistic treatment of transition slaved and transition representative atoms. Such an atomistic treatment together with a full or cutoff sampling allows non-local transition elements containing these transition entities to transmit inhomogeneity. Different force formulations for transition representative atoms and pure local representative atoms allow the local transition elements to resolve non-local and local mismatches. The method presented herein is validated by force calculations in an unstressed perfect crystal as well as an unrelaxed grain boundary model. A nanoindentation simulation in 3D is conducted to demonstrate the accuracy and efficiency of the proposed method.

Keywords: quasicontinuum; transition; atomistic model; finite elements

1. Introduction

Atomistic modeling has been used to address a wide variety of deformation processes in solids recently (Chen *et al.* 2008, Chan *et al.* 2011, Lai and Chen 2013, Chen and Lee 2010, Jeong *et al.* 2011, Shen 2013, Teng *et al.* 2011, Wang *et al.* 2013, Zhao and Aluru 2008). The advantage of fully atomistic modeling is its capability to provide desirable resolution that accounts for highly inhomogeneous deformations caused by lattice defects in materials. On the other hand, the weakness of the atomistic approach is that it must incorporate a significant number of redundant degrees of freedom for atoms that are relatively far away from the defects. Thus, the application of fully atomistic modeling is limited by available computing resources. This limitation often prevents researchers from modeling realistic structures for sizes that exceed a few hundred nanometers.

*Corresponding author, Professor, E-mail: dchen@ntu.edu.tw

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