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A continuum computational method incorporating atomic interactions of materials

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Summary

Bridging the atomic and continuous analyses is an important aspect in multi-scale mechanics. This paper develops a computational method to integrate the atomic potential of a material with the finite element method. The novelty of this method is that the strain energy is calculated from the atomic potential without the assumption in the Cauchy-Born rule that deformation in a virtual atomic cell is homogeneous. In our new method, the virtual atomic cell deformation is interpolated according to the continuum displacements constructed associated with the shape functions. The applications of the method to single crystal Si and Ge bars under uniaxial tension and compression show that the Young's moduli in the <100> direction obtained are in good agreement with the experimental measurements and MD simulations in the literature. Moreover, the simulated material response to tension and compression is qualitatively consistent with the interatomic interaction.