Determining Material Constants in Nonlocal Micromorphic Theory through Phonon Dispersion Relations

Xiaowei Zeng*, James D. Lee, Youping Chen

Department of Mechanical and Aerospace Engineering
School of Engineering and Applied Science
The George Washington University, 801 22nd street, NW, Washington, DC 20052
xwzeng@gwu.edu

Phonon dispersion relation is an essential feature representing the atomic structure and atomic motions in crystal. It can be calculated from atomic force by a discrete atomic model. The analog of atomic force is the constitutive relations in the continuum theory, which serve to distinguish one material from another. It follows that the phonon dispersion relations can be also calculated through the constitutive relations of a material by a continuum model if the model can manifest the dynamics of atoms in crystals, and hence provides a bridge to link the interatomic force to the constitutive relations.

This paper aims to determine the material constants in nonlocal micromorphic theory through phonon dispersion relations. The nonlocal constitutive relations for isotropic elastic solids in micromorphic theory are derived. The numerical algorithm to determine the material constants is presented. The material constants for single crystal silicon and diamond in local and nonlocal micromorphic theory are determined by fitting the phonon dispersion relations from atomistic calculations or experimental measurements. The local miromorphic theory can only fit the dispersion relation faithfully in half Brillouin zone, while it is found that the nonlocal solutions lead to dispersion relations that are in quite good agreement with the lattice dynamical results throughout the entire Brillouin zone. The applicability of nonlocal micromorphic theory has been discussed.

Keywords: micromorphic, nonlocal, optimization