

Abstract Submitted
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Fast full-spectrum phonon calculations for large lattices by Bloch mode synthesis DIMITRI KRATTIGER, MAHMOUD HUSSEIN, University of Colorado Boulder — Computation of thermal properties from lattice dynamics models involves integration over all phonon modes in the system. These phonon modes can be found by solving an eigenvalue problem. For periodic nanostructures, the degrees of freedom in the system may number in the thousands or even millions, resulting in a very expensive computational problem. Bloch mode synthesis is a recently developed model reduction technique whereby the size of the eigenvalue problem is greatly decreased. Similar to sub-structuring techniques, this method separates the domain into interface and interior degrees of freedom, and performs a modal reduction on the interior. Meanwhile the interface is represented using a set of static constraint modes. In the current work, this reduction is modified by using dynamic constraint modes so that it can be applied at higher frequency ranges. This effectively breaks up the large eigenvalue problem into many small eigenvalue problems resulting in large computational savings.

Dimitri Krattiger
University of Colorado Boulder

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