

Abstract Submitted
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Tight binding calculations of vibrational and thermal properties of amorphous silicon MICHAEL MEHL, Naval Research Laboratory, JOSEPH FELDMAN, DIMITRIS PAPACONSTANTOPOULOS, Naval Research Laboratory and George Mason University, NOAM BERNSTEIN, Naval Research Laboratory — By displacing atoms by different amounts and computing atomic forces within the NRL tight binding method we obtain all second order (harmonic) and some third order (anharmonic) coupling constants of a 1000 atom TB-relaxed Wooten CRN model of amorphous silicon. The harmonic force constant results allow us to study various properties including vibrational density of states, dynamic structure factors, specific heat and thermal conductivity within Kubo theory. We shall present results of these applications and compare to experiment and previous work based on the Stillinger Weber potential.

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