

Abstract Submitted
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Vibrational structure of the alkali metal surfaces R. WILSON, D.M. RIFFE, Utah State University — Many physical properties of solids are phonon dependent. While numerous theoretical and experimental investigations have successfully characterized bulk vibrational structure, further characterization of surface phonons is needed. The behavior of surface phonons is important to the understanding of nano-structures, the interpretation of experimental measurements used to study solids, and the understanding of a variety of physical phenomena that solids exhibit. We present the calculation of vibrational modes on the (110) and (100) of alkali metal surfaces with the use of an Embedded Atom Method (EAM) interatomic potential. Vibrational dependent properties in the bulk that are calculated by the EAM potential are in good agreement with experiment, providing credibility to the EAM potential's accuracy. Surface properties such as entropy, specific heat, vibrational density of states, and Debye temperatures are calculated from the vibrational modes. The surface phonons are found to be highly polarized, resulting in anisotropic thermal behavior at and near the surface. A database of bulk and surface Debye temperatures is being created as a resource.

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