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An analytical bond-order potential for the cadmium telluride binary system

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ABSTRACT

CdTe and $Cd_{1-x}Zn_xTe$ are the leading semiconductor compounds for both photovoltaic and radiation-detection applications. The performance of these materials is sensitive to the presence of atomic scale defects in the structures. To enable accurate studies of these defects using modern atomistic simulation technologies, we develop a high-fidelity analytical bond-order potential for the CdTe system. This potential incorporates primary (σ) and secondary (π) bonding and the valence-dependence of the heteroatom interactions. The functional forms of the potential are directly derived from quantum-mechanical tight-binding theory under the condition that the first two and first four levels of the expanded Green's function for the σ- and π- bond-orders, respectively, are retained. The potential parameters are optimized using iteration cycles that include first fitting properties of a variety of elemental and compound configurations (with coordination varying from 1 to 12) including small clusters, bulk lattices, defects, and surfaces, and then checking crystalline growth through vapor deposition simulations. It is demonstrated that this CdTe bond-order potential gives structural and property trends close to those seen in experiments and quantum-mechanical calculations, and provides a good description of melting temperature, defect characteristics, and surface reconstructions of the CdTe compound. Most importantly, this potential captures the crystalline growth of the ground-state structures for Cd, Te, and CdTe phases in vapor deposition simulations.

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Bio: D.K. Ward has been a post doc at Sandia National Lab in Livermore, CA, since 2010. He received his BS (Engineering/Mechanical) from Colorado School of Mines in 2001. He then earned his Ph.D. from Brown University (Solid Mechanics) working under W.A. Curtin in 2007. His thesis centered on Al/Si nanocomposites and size-scaling of Au nanoasperity compression. Following graduate school he spent two years as a post doc in the Center for Advanced Vehicular Systems (CAVS) at Mississippi State University. While at CAVS, Dr. Ward explored deformation mechanisms of polyethylene, polycrystalline damage, and hydrogen embrittlement. Dr. Ward's current research continues to focus on atomistic modeling of a range of materials including metals, plastics, and semiconductors, with the purpose of understanding fundamental mechanisms responsible for nano/micro scale behavior.