(Prepared for SPIE 2011 Photonic Devices + Applications; San Diego, CA, August 21-25, 2011)
SAND2011-1600C

Bond order potential-based molecular dynamics model for CZT melt-growth simulations

X. W. Zhou, D. K. Ward, B. M. Wong, and F. P. Doty

Sandia National Laboratories, Livermore, California 94550, USA

CdTe-based $Cd_{1-x}Zn_xTe$ (CZT) alloy compound is the leading semiconductor for γ-ray detection. The wide-spread deployment of the CZT detectors, however, is currently limited by the high costs of detector-grade materials due to their low manufacturing yields. The formation of defects such as grain boundaries, tellurium inclusions / precipitates, and dislocations during crystal growth has been the limiting factor for the property non-uniformity and the resulting low manufacturing yields. The problem is that while these defects can easily form and are prevalent in the material, their formation mechanisms are not well understood and hence they are difficult to remove. To enable the study of correlation between growth conditions and defect generation on a fine scale using high fidelity molecular dynamics simulations, we have been developing an analytical bond-order potential for the CZT system. The functional forms of the potential were directly derived from the tight-binding theory under the condition that the first two levels of the expanded Green function for the σ- and π- bond orders are retained. The potential incorporates primary (σ) and secondary (π) bonding and the valence-dependence of the heteroatom interactions. The potential parameters are parameterized considering properties of a variety of elemental and compound configurations (with coordination varying from 1 to 12) including small clusters, bulk lattices, defects, and surfaces. As a first stage for modeling CZT, preliminary parameterization has been completed for the CdTe system. It is demonstrated that this CdTe bond-order potential not only predicts a structural and binding energy trend close to that seen in experiments and ab initio calculations, but also accurate melting temperatures for equilibrium Cd, Te, and CdTe phases and various CdTe (001) surface reconstructions. Most importantly, we have validated this potential by demonstrating its ability to predict the liquid phase growth of zinc-blende CdTe crystals. The emergence of such a BOP-based method begins to enable defect formation mechanisms in CZT crystals to be studied at a fidelity level comparable to ab initio methods and a scale level comparable to empirical molecular dynamics simulation methods.

This work is supported by the NNSA/DOE Office of Nonproliferation Research and Development, Proliferation Detection Program, Advanced Materials Portfolio. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.