Atomistic Simulations of Cadmium Telluride: Toward Understanding the Benefits of Microgravity Crystal Growth

J.J. Derby (PI) and J.R. Chelikowsky (Co-PI)
Department of Chemical Engineering and Materials Science
151 Amundson Hall
421 Washington Avenue, S.E.
Minneapolis, MN 55455-0132

Telephone: (612) 625-1313
Fax: (612) 626-7246
E-mail: derby@tc.umn.edu, jrc@msi.umn.edu

Introduction and Objectives

Progress in crystal growth on earth or in space will depend on a more fundamental understanding of the important coupling between atomistic-scale processes which control the properties of grown crystalline material and the macroscopic transport conditions imposed by the growth system. Our long-term goal is to understand the mechanisms which influence crystal quality through the hierarchy of length and time scales relevant to these atomistic-scale and macro-scale processes. The immediate goal of the research summarized here is to employ atomistic simulation to understand better the melt growth of cadmium telluride (CdTe) and its alloy cadmium zinc telluride (CdZnTe). These materials are employed in a variety of technologically important electronic and electro-optical devices; however, the growth of high-quality, large-area single crystal substrate has proven to be extremely difficult under terrestrial conditions. We seek to obtain a more fundamental understanding of the properties of cadmium telluride so that the physical mechanisms responsible for growth can be elucidated. A secondary objective of our work is the prediction of high-temperature thermophysical properties of liquid and solid CdTe.

Relationship to Microgravity Research

Recent growth experiments of $Cd_{0.96}Zn_{0.04}Te$ in a microgravity environment aboard USML-1 resulted in material which was far superior in structural perfection compared to earth-grown material under similar conditions. These dramatic results were attributed to the elimination of hydrostatic pressure from the melt column overlaying the crystal due to microgravity conditions, thereby reducing the hoop stresses that occur in a crystal as it grows and cools. In addition, it was speculated that the near absence of hydrostatic pressure allowed for the melt to solidify with minimal wall contact, thereby eliminating deleterious wall interactions. We will utilize atomistic simulation to understand the dynamics of the liquid/solid interface and of the solid material under the stress conditions corresponding to micro-gravity and terrestrial conditions. The work to be performed in this project will support current microgravity research on the melt growth of CdTe compounds and will provide for a quantitative, unambiguous method to understand the subtle effects of microgravity in these systems.

The primary thrust of this work will be to clarify the role of microgravity in interpreting the USML-1 results described above; however, this work promises to support future microgravity research in other substantial ways. Atomistic simulations will provide predictions of the high-temperature thermophysical properties of CdTe and its alloys. Accurate high-temperature properties are needed for reliable materials processing models, but such data are extremely difficult to obtain from experimental measurements (many of which have been undertaken in microgravity environments). The prediction of these properties using atomistic simulation clearly complements ongoing and future microgravity process modeling and experimental property measurement efforts. Another

likely benefit from this work is that a more complete understanding of the structure of molten CdTe and alloys will aid the development of seeding procedures for melt growth. For earth-based processes, reliable seeding techniques have not yet been developed for these materials, yet such procedures have been identified as one of the most needed process improvement to increase yields. Undoubtedly, as further microgravity experiments on the melt growth of CdZnTe are performed, seeded growth experiments will be desired and the knowledge obtained from atomistic simulations will be invaluable.

Methodology and Results

We have successfully employed *ab initio* pseudopotentials to compute the electronic structure of solid and liquid CdTe. Subsequent work focused on performing first principles molecular dynamics simulations on the liquid state using interatomic forces between atoms to calculate the atomic trajectories and integrate the equations of motions to simulate the liquid. The liquid was modeled by considering a 64 atom unit cell with periodic boundary conditions; the atoms were randomly place in this cell and initially heated to a very high temperature. After cooling the system to a temperature slightly above the melting temperature, we analyzed the resulting liquid.

We have determined the pair correlation function, the self-diffusion of the Cd and Te atoms, and have performed an analysis of the liquid structure. We compared the theoretical results for the pair correlation function to experimental x-ray and neutron work. Our initial comparisons are quite encouraging; the predicted and experimental distributions are quite similar. Likewise, our computed diffusion coefficients are consistent with experiments.

We have submitted a manuscript entitled "*Ab Initio* Molecular Dynamics Simulation of Liquid CdTe and GaAs: Semiconducting versus Metallic Behavior" to *Physical Review Letters*. All semiconductors of IV row, such as silicon, and III-V materials, such as gallium arsenide, assume metallic behavior when melted. This is in contrast to some II-VI semiconductors such as CdTe which retain their semiconducting behavior in both the liquid and the solid state. In order to understand this difference, we have performed *ab initio* molecular dynamics simulations of liquid GaAs and CdTe. Using the Kubo-Greenwood formalism, we predict the conductivity of both liquids and confirm the differences observed experimentally. We relate the conductivity differences between II-VI and III-V semiconductors to strong structural differences occurring within the melt.