Thermophysical Property Measurements of Te-Based II-VI Semiconductor Compounds

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Compound II-VI semiconductor components are increasingly employed in a wide variety of electronic and optical devices. However, the yield of device quality material varies between solidification runs and this limits their ultimate commercial utility (i.e., yields of 5-10% for active devices is considered excellent). Advances in our understanding and control of materials preparation for devices has benefited from numerical modeling efforts. In particular, insight into bulk transport and segregation processes has been obtained. However, for these modeling efforts to yield further guidance, and consequently, improvements in device yields, accurate data for molten state diffusivities and thermophysical properties, and, in particular, their temperature dependence, is essential. At present such data is either missing or poorly defined.

The experimental determination of transport properties such as diffusivities and conductivities is often contaminated by buoyancy-driven convective effects. The accurate determination of transport properties requires convective flow velocities to be eliminated or significantly suppressed. This is generally not possible under terrestrial conditions. While it can be argued that mass diffusivity measurement techniques such as nuclear magnetic resonance and inelastic neutron scattering, that probe rapid molecular motion, are insensitive to convective contributions, they are not as precise as macroscopic, averaging techniques. However, all macroscopic measurement techniques yield diffusivity data prone to be contaminated by gravity-driven convection. The use of narrow capillaries to suppress convective transport has suggested poorly understood wall effects. Magnetic fields, widely used for suppressing convection in conducting liquids, modify the diffusive motion itself. Earlier liquid (metal) diffusion studies conducted on spacecraft have demonstrated the gain in precision resulting from the drastic reduction of convection in a low-gravity environments. However, by comparison with ground-based experiments, the most recently reported low-gravity data using a shear-cell technique appear rather inaccurate.

Thermal diffusivity measurements in melts are also prone to be contaminated by convective contributions. The use of small measuring volumes increases the likelihood that asymmetries and imperfections in the measurement apparatus itself leads to errors. The use of larger cell volumes on the other hand is prone to result in convective contamination. These problems can be especially troublesome with II-VI semiconductors, since their thermal conductivity is smaller than that of typical container materials. Levitated drop techniques offer little relief of this problem due to the high vapor pressure of II-VI compounds. Modeling of these convective contributions is at best problematic since the assumptions for estimating or modeling these contributions depends on ground-based data already influenced by convection. Again, magnetic fields, widely used for suppressing convection in conducting liquids, can be expected to modify the diffusive motion

itself. Earlier liquid thermal conductivity/diffusivity studies conducted on spacecraft have demonstrated the gain in precision, and lower absolute values, resulting from the drastic reduction of convection in a low-gravity environments. Hence, there is also a need for well defined thermal diffusivity studies under low gravity.

Our group has developed a novel molten-metal diffusivity measurement approach under NASA sponsorship. This approach is particularly suited to the limited availability of experiment time on space flights. Diffusivities are deduced *in-situ* and in real-time from consecutive concentration profiles obtained from radioisotope emission using a multiple detector arrangement. The use of a novel algorithm for diffusivity evaluation permits measurements at several temperatures in the same sample and, thus, coverage of a wide temperature range with a few samples. Furthermore, with elements that simultaneously emit high and low energy photons, which we have predominately chosen for this research, discrimination of photon energy will permit the distinction of transport near the capillary wall and in the bulk of the fluid. A single temperature hardware unit utilizing this approach to measure diffusion coefficients in molten indium metal has flown under NASA sponsorship on a MIR flight. The self-diffusivity values we have measured both on the ground and in space are among the lowest values reported for this material.

Diffusivity and thermophysical properties for the tellurium based II-VI binary semiconductors (CdTe, HgTe and ZnTe) have been studied quite extensively in the solid state. However, for the molten state only few values exist, and the temperature dependence is practically unknown. We propose to extend our presently employed “novel” diffusivity technique to the

- measurement of binary- and (selected) impurity-diffusivity in melts of Te-based II-VI compounds.

In addition, we will measure the following interrelated thermophysical parameters:

- density change on melting and the volume expansion coefficient of the melt for pure and doped materials,
- melt thermal conductivity and thermal diffusivity.

The proposed four-year program includes the following tasks:

- Construction of hardware for measurements of the diffusivity of the binary components and selected impurities.
- Design and construction of hardware for the determination of thermal and solutal volume expansion coefficient.
- Design and construction of hardware for the determination of thermal conductivity/ diffusivity.
- Numerical modeling efforts in support of the thermal conductivity/diffusivity measurements.
- Analytical-numerical modeling to develop a three-dimensional model of X-ray self-absorption.
- Construction and testing of flight hardware for the measurement of binary component and/or impurity diffusivity measurements at multiple temperatures with a single sample.
- Construction and testing of flight hardware for the determination of thermal conductivity or diffusivity.