Thermophysical Property Measurements of Molten Semiconductors in 1-g and Reduced-g Condition

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Understanding and controlling the formation kinetics of a variety of crystal imperfections such as point defects, non uniform distribution of doping atoms, and impurity atoms in the growing crystals are very important. To achieve this objective, a theoretical (numerical) modeling of crystal growth process is an essential step. In order to obtain reliable modeling result, the input parameters (i.e., various thermophysical parameters) must be accurate. Importance of accurate thermophysical properties of semiconductors in crystal growth cannot be overly emphasized. The total hemispherical emissivity, for instance, has a dramatic impact on the thermal environment. It determines the radiative emission from the surface of the melt determining to a large extent the profile of the solidified crystal. In order to understand convection and turbulence in the melt, viscosity becomes important parameter. The liquid surface tension determines the shape of the liquid-atmosphere interface near the solid-liquid-atmosphere triple point. Currently used values for these parameters are rather inaccurate, and this program intends to provide more reliable thermophysical properties. Thus, the objective of this program is in the accurate measurements of various thermophysical properties which can be reliably used in the modeling of various crystal growth processes.

In this program, thermophysical properties of molten semiconductors, such as Si, Ge, Si-Ge, and InSb will be measured as a function of temperature using the High Temperature Electrostatic Levitator at JPL. Each material will be doped by different kinds of impurities at various doping level. Thermophysical properties which will be measured include: density, thermal expansion coefficient, surface tension, viscosity, specific heat, hemispherical total emissivity, and perhaps electrical and thermal conductivities.

Many molten semiconductors are chemically reactive with crucibles so that dispersed impurities in the melts tend to substantially modify the properties of pure semiconductors. Sample levitation done in a vacuum clearly helps maintain the sample purity. However, in the 1-g environment, all gravity-caused effects (such as convection, sedimentation, and buoyancy) are still present in the sample. In addition, large forces needed to levitate the sample in the presence of gravity can cause additional flows in the melt. The High Temperature Electrostatic Levitator (HTESL) that is being used for the present research is a recent development, and little is known about the flows induced by the electrostatic forces. In this ground-based program, we will define the limits of HTESL technology as various thermophysical properties of molten semiconductors are measured.

Progress

Progress has been made in the measurement of thermophysical properties of molten silicon and germanium. In molten silicon, the density, the ratio between the specific heat and the spherical

total emissivity, the surface tension, and the viscosity have been measured. The quadratic nature of the liquid density as a function of temperature was observed, indicating a certain short range ordering which might be forming as the liquid undercooled deeply. Unlike most pure metals, nonlinear increase of the specific heat in the undercooling silicon has also been repeatedly observed. Again, formation of some orders must be responsible to such nonlinear behavior. Measured silicon surface tension showed reasonable agreement with the literature values. However, an uncontrollable sample rotation which set in during the sample heating process could not be controlled. The drop resonance frequency should depend on the rotation rate; therefore, it was important to develop a sample rotation control capability to ensure the rotation frequency falls within an acceptable range. We have succeeded in developing the rotation control system, and integrated it in the JPL HTESL. We are ready to revisit the surface tension and viscosity measurements of molten silicon with the new capability.

We have investigated the thermophysical properties of molten germanium. Pure germanium was melted during levitation and measured the density, the ratio of heat capacity to hemispherical total emissivity, the surface tension, and the viscosity. Using the newly developed non-contact method, the electrical resistivity of germanium around the melting temperature was determined. From the measured resistivity, the thermal conductivity of germanium was determined using the Wiedemann-Franz-Lorenz relationship. Considering the fact that the thermal conductivity is one of the transport properties which is susceptible to gravity induced flows, this indirect approach to the thermal conductivity from the electrical conductivity measurement may have an important implication in terms of increased accuracy of thermal conductivity.

Evidences are being accumulated in terms of the range of liquid viscosity which can be measured in the 1-g environment using the HTESL. At their melting temperatures, both molten silicon and germanium show viscosities in the range of 1 mPa•sec which seems to be just about the limiting viscosity in 1-g using the HTESL. Viscosity measurement method relies on the measurement of the damping time constant of a freely oscillating drop. On the other hand, levitation of a melt in a 1-g environment requires application of a strong controlled electrostatic field to counter the weight. Any interference of free decay process by the levitation control force can modify the decay process, therefore, the decay constant. This problem will be more severe lower the viscosity.

The knowledge of spectral emissivity of sample materials at the wavelength of pyrometer is important to know the true temperature of the sample. Without this capability, the need of a known reference temperature is essential, and a further assumption on constant spectral emissivity has to be made. In an environment where such reference point is not available, and the constant emissivity assumption is under suspect, temperature determination of a given alloy becomes quite uncertain. For this reason, we have purchased and integrated in the HTESL a commercial instrument which measures the spectral emissivity that will help determine the true temperature. Also installed was a 100 W YAG laser which would allow the sample temperature measurement even during the sample heating cycle. This high power laser will be able to heat a sample higher than 2000 °C.