Vapor Growth of ZnSe-based Compound Semiconductors in Low Gravity environment on International Space Station

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Six low-gravity experiments of crystal growth of ZnSe-based compound semiconductors by physical vapor transport (PVT) are scheduled to be processed inside Low Gradient Furnace (LGF) on Materials Science Research Rack (MSRR) in Material Science Laboratory (MSL) on International Space Station (ISS) starting from February 27th, 2023. The flight samples consist of three unseeded growths of ZnSe, Cr-doped ZnSe and ZnSeTe as well as growth of ZnSe on top of three single crystal ZnSe seeds with orientation of (100), (110) and (111). The main scientific objective of the flight experiments is to establish the effects of gravity-driven fluid flows on Earth to (i) the non-uniform incorporation of impurities and defects and (ii) the deviation from stoichiometry observed in the grown crystals caused by growth interface fluctuations and evolution as the results of buoyancy-driven convection and irregular fluid-flows. The investigation will also evaluate the effects of gravity on the PVT process by examining (i) the growth kinetics on various seed orientations, (ii) the dopant segregation and distribution in the Cr doped ZnSe, and (iii) the compositional segregation and distribution in the ternary ZnSeTe crystal grown by PVT. Additionally, from X-ray diffraction/topography and by measuring the density and distribution of various crystalline defects it will assess the self-induced strain effects developed during processing at elevated temperatures caused by the weight of the crystals.

During the ground-based preparations, the following tasks have been accomplished:

- Establish the thermodynamic properties of the ZnSe binary and related ternary systems by measuring the partial pressures of the vapor phase coexisting with the condensed phases and perform phase diagram calculations for comparison.
- Evaluate the effects of gravity-driven convection in the growth process by performing experiments under various vapor transport orientations relative to gravity vector, i.e., horizontal, vertically stabilized and destabilized configurations.
- Establish a quantitative correlation between growth parameters and the characteristics and properties of the grown crystals by characterizing the crystals using a variety of techniques.
- Evaluate the fundamentals of the current theories on vapor transport and crystal growth kinetics by performing *in-situ* and real-time monitoring techniques during growth.
- Develop a one-dimensional diffusion limited theory of mass transport and two- and three-dimensional numerical simulations of both mass transport and heat transfer and thus establish the microgravity requirements for the flight experiments and to predict the characteristics of the grown crystals such as the solid-vapor interface shapes… etc. and establish a fundamental understanding of the crystal growth process from the comparison with experimental results.