MODELS OF MASS TRANSPORT DURING MICROGRAVITY CRYSTAL GROWTH OF ALLOYED SEMICONDUCTORS IN A MAGNETIC FIELD

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Alloyed semiconductor crystals, such as germanium-silicon (GeSi) and various II-VI alloyed crystals, are extremely important for optoelectronic devices. Currently, high-quality crystals of GeSi and of II-VI alloys can be grown by epitaxial processes, but the time required to grow a certain amount of single crystal is roughly 1,000 times longer than the time required for Bridgman growth from a melt. Recent rapid advances in optoelectronics have led to a great demand for more and larger crystals with fewer dislocations and other microdefects and with more uniform and controllable compositions. Currently, alloyed crystals grown by bulk methods have unacceptable levels of segregation in the composition of the crystal. Alloyed crystals are being grown by the Bridgman process in space in order to develop successful bulk-growth methods, with the hope that the technology will be equally successful on earth. Unfortunately some crystals grown in space still have unacceptable segregation, for example, due to residual accelerations. The application of a weak magnetic field during crystal growth in space may eliminate the undesirable segregation. Understanding and improving the bulk growth of alloyed semiconductors in microgravity is critically important. The purpose of this grant to to develop models of the unsteady species transport during the bulk growth of alloyed semiconductor crystals in the presence of a magnetic field in microgravity. The research supports experiments being conducted in the High Magnetic Field Solidification Facility at Marshall Space Flight Center (MSFC) and future experiments on the International Space Station.

For alloyed semiconductors, the density differences due to compositional variations in the melt are very large. In germanium-silicon (GeSi), for example, the mole fraction of germanium may vary from 0.95 in the melt which has not yet received any rejected germanium to 0.99 near the interface, and this compositional difference corresponds to a density difference of nearly 300 kg/m^3. In a frequently used extension of the Boussinesq approximation, the melt density is assumed to vary linearly with both the temperature and mole fraction of either species. In this approximation, the magnitudes of the density difference and of the resultant buoyant convection associated with the temperature variation or with the compositional variation are characterized by $\beta_T(\Delta T)_o$ and $\beta_C C_o$, respectively, where β_T and β_C are the thermal and compositional coefficient of volumetric expansion, while $(\Delta T)_o$ and C_o are the characteristic radial temperature difference and the initially uniform mole fraction of the species, i.e. of silicon in the GeSi melt. For GeSi with $(\Delta T)_o$=10 K and C_o=0.02, the characteristic ratio of the buoyant convection driven by thermal variations to that driven by compositional variations is $\beta_T(\Delta T)_o/\beta_C C_o$=0.2. While the thermally-driven buoyant convection is probably not negligible, particularly far from the crystal-melt interface where compositional variations are small, the compositionally-driven buoyant convection or soluto-convection is dominant particularly near the interface.

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During the Bridgman growth of alloyed semiconductor crystals, the application of magnetic fields have shown great promise. For example, Watring and Lehoczky [1] have shown that the radial variation between the maximum and minimum concentrations can be decreased by more than a factor of three with the application of a 5 T magnetic field, arising because the magnetic field retards the sinking of the heavier melt to the center of the ampoule, resulting in less radial segregation. Ramachandran and Watring [2] reported a reduction in the radial segregation in all of their samples which were grown in a magnetic field.

The numerical treatment of transient species transport is difficult because (1) there are extreme differences between the time scales for the diffusions of internal energy, momentum and species, and (2) there are thin species-diffusion or viscous boundary layers for every value of the magnetic field strength. Therefore, the simultaneous time integration of the full Navier-Stokes, internal energy, and species transport equations must always have a very fine spatial grid and a very small time step so that simulating the entire crystal growth process is challenging. Our models involve the use of asymptotic models, which complement the numerical solutions of the full equations, in order to reduce the number of computations that are needed to accurately treat the entire growth process. Our simulations provide physical insight into the transport processes and can be used to systematically search over all possible combinations of controllable process parameters in order to determine the optimal processes which minimize segregation in the crystal.

To date, we have developed models [3,4] which treat the thermally-driven and compositionally-driven buoyant convections or solutal convection during the Bridgman or vertical gradient freezing growth alloyed semiconductor crystals with various orientations of an externally-applied steady magnetic field. The primary objective of this grant is to develop models which investigate the effects of the microgravity environment on segregation in the alloyed crystal grown in a magnetic field. Future research will be focused on applying our methods to treat solutal convection during the vertical gradient freezing of alloyed semiconductor crystals in a magnetic field in space. The effects of all three components of the residual acceleration, namely, the steady (DC) acceleration, g-jitters and spikes, eventually need to be investigated. The models would involve using asymptotic approximations which are appropriate for the reduced convective flows in microgravity and for the magnetic fields that will be used on the International Space Station.

Other research projects which have been supported by this grant include analytical and numerical modelling of (1) melt motions during floating-zone growth of high-purity silicon crystals in steady and rotating magnetic fields [5,6], (2) dopant transport during horizontal Bridgman growth of semiconductors in steady magnetic fields [7-9], and (3) dopant transport during liquid-encapsulated growth of compound semiconductor crystals in a magnetic field [10-14].

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References

1. D. A. Watring and S. L. Lehoczk, 1996, "Magneto-hydrodynamic Damping of Convection during Vertical Bridgman-Stockbarger Growth of HgCdTe," *Journal of Crystal Growth*, vol. 167, no. 3/4, pp. 478-487, October 1996.

2. N. Ramachandran and D. A. Watring, "Convection damping by an axial magnetic field during growth of HgCdTe by vertical bridgman method," AIAA 35th Aerospace Sciences Meeting and Exhibit, Reno, NV, AIAA Paper #97-0450, January 1997.
3. N. Ma, "Solutal convection during melt growth of alloyed semiconductor crystals in a steady magnetic field," AIAA 40th Aerospace Sciences Meeting and Exhibit, AIAA Paper #2002-1113, Reno, NV, January 2002.
4. M. V. Farrell and Nancy Ma, "Solutal convection during semiconductor crystal growth. Axial versus transverse magnetic fields," ASME International Mechanical Engineering Congress and Exposition, New Orleans, LA, November 2002, in press.
5. N. Ma, J. S. Walker, A. Lüdge and H. Riemann, "Silicon floating-zone process with a weak transverse magnetic field and crystal rotation," *Journal of the Electrochemical Society*, vol. 147, no. 9, pp. 3529-3534, September 2000.
6. N. Ma, J. S. Walker, A. Lüdge and H. Riemann, "Combining a rotating magnetic field and crystal rotation in the floating zone process with a needle eye induction coil," *Journal of Crystal Growth*, vol. 230, no. 1/2, pp. 118-124, August 2001.
7. J. M. Hirtz and N. Ma, "Dopant transport during semiconductor crystal growth. Axial versus transverse magnetic fields," *Journal of Crystal Growth*, vol. 210, no. 4, pp. 554-572, March 2000.
8. J. M. Hirtz and N. Ma, "Scaleability of dopant composition in semiconductor crystals grown by the Bridgman process in the presence of magnetic fields," AIAA 38th Aerospace Sciences Meeting and Exhibit, AIAA Paper #2000-1019, Reno, NV, January 2000.
9. T. E. Hockenhull and N. Ma, "Dopant transport during semiconductor crystal growth in space with a steady magnetic field," *Magnetohydrodynamics*, vol. 36, no. 3, pp. 289-296, 2000.
10. N. Ma, D. F. Bliss and G. G. Bryant, "Segregation during magnetically-stabilized liquid-encapsulated growth of compound semiconductor crystals," ASME *Proceedings of the Fluids Engineering Division*, FED-vol. 253, pp. 215-221, Orlando, FL, November 2000.
11. N. Ma and J. S. Walker, "Inertia and thermal convection during crystal growth with a steady magnetic field," AIAA *Journal of Thermophysics and Heat Transfer*, vol. 15, no. 1, pp. 50-54, January-March 2001.
12. J. L. Morton, N. Ma, D. F. Bliss and G. G. Bryant, "Diffusion-controlled dopant transport during magnetically-stabilized liquid-encapsulated Czochralski growth of compound semiconductor crystals," ASME *Journal of Fluids Engineering*, vol. 123, no. 4, pp. 893-898, December 2001.
13. M. V. Farrell and N. Ma, "Coupling of buoyant convections in boron oxide and a molten semiconductor in a vertical magnetic field," ASME *Journal of Heat Transfer*, vol. 124, no. 3, 2002.
14. J. L. Morton, N. Ma, D. F. Bliss and G. G. Bryant, "Dopant segregation during liquid-encapsulated Czochralski crystal growth in a steady magnetic field," *Journal of Crystal Growth*, in press.