Dopant segregation in semiconductor crystal growth due to stochastic g-jitter in microgravity

X. Ruiz,[a] P. Bitlloch,[b] L. Ramírez-Piscina,[c] J. Casademunt[b]
IEEC Institut d'Estudis Espacials de Catalunya, Barcelona, Spain

In microgravity environments there exist residual accelerations (g-jitters) that typicaly contain a broad spectrum of frequencies. These accelerations can be modelled as stochastic processes, and can have a relevant influence in fluid systems. In this work[1] we have quantitatively addressed the effects of a generic stochastic g-jitter into the quality of semiconductor crystals grown in realistic directional solidification setups. In particular we evaluate, by means of direct numerical simulations and by a simplified model, the dopant segregation effects due to thermosolutal convection as a function of the parameters characterizing the statistics of the stochastic force.

Simulations are specified for material parameters of two doped semiconductors (Ge : Ga and GaAs : Se) in realistic conditions of actual microgravity environments. The numerical simulation of the growth process involves the resolution of the time dependent transport equations in the melt ahead of the solidification front with the appropriate boundary conditions at the moving interface. We have considered a Boussinesq, incompressible fluid, and we have neglected deformations of the interface. For the stochastic gravity we have used narrow-band noise, which is a stochastic process characterized by its amplitude G, a temporal correlation τ, and a dominant frequency Ω, given by the main peak of its power spectrum

$$P(\omega) = \frac{G^2\tau}{2\pi}\left(\frac{1}{1+\tau^2(\Omega+\omega)^2} + \frac{1}{1+\tau^2(\Omega-\omega)^2}\right). \quad (1)$$

Additionaly we have considered deterministic oscillations of the same frequency.

We have explored the response of the system for the two semiconductors considered for different thermal profiles of the setup and different amplitudes of the stochastic signal. As a general result of the direct simulations, the response of the system is very weak, and essentialy linear in the amplitude of the g-jitter.

In addition, we have developed a simplified model of the problem based on linear response theory that projects the dynamics into very few effective modes. The model involves two effective time scales, one from viscous dissipation and one from solutal diffusion. Those can be fitted from the simulation of a single convenient case, and on the basis of linear response theory, the model can be extended to arbitrary signals.

Careful analysis of the model predicts that the response of the system is strongly dominated by the low-frequency part of the g-jitter spectrum. This was confirmed by the numerical results of the complete model. We have also shown that the model captures remarkably well the segregation effects for an arbitrary time-dependent acceleration of small amplitude, while it implies an enormous reduction of computer demands. This model could be helpful to analyze results from real accelerometric signals and also as a predictive tool for experimental design.

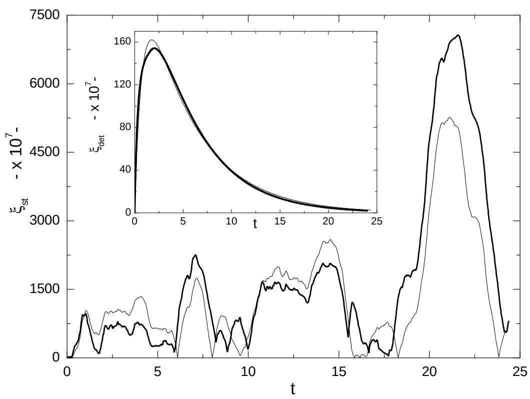

FIG. 1. Transversal segregation parameter as a function of time, for GaAs : Se, obtained from both the complete simulation (thick line) and the integration of the simple model (thin line) by employing the same noisy signal. Inset: nonlinear fitting of the model to the simulation of the complete system for the deterministic case, which is used to obtain the value of the three parameters needed in the noisy case.

[a] Dept. Química Física i Inorgànica, Universitat Rovira i Virgili. Tarragona, Spain.
[b] Dept. Estructura i constituents de la Matèria, Universitat de Barcelona. Barcelona, Spain.
[c] Dept. Física Aplicada, Universitat Politècnica de Catalunya. Barcelona, Spain.
[1] X. Ruiz, P. Bitlloch, L. Ramírez-Piscina and J. Casademunt, *Impact of stochastic accelerations on dopant segregation in microgravity semiconductor crystal growth*, submitted to Journal of Crystal Growth.