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Impact of stochastic accelerations on dopant segregation in microgravity semiconductor crystal growth

X. Ruiz [a,d,*], P. Bitlloch [b], L. Ramírez-Piscina [c,d], J. Casademunt [b,d]

[a] Departament de Química Física i Inorgànica, Universitat Rovira i Virgili, Tarragona, Spain
[b] Departament de Estructura i Constituents de la Matèria, Universitat de Barcelona, Barcelona, Spain
[c] Departament de Física Aplicada, Universitat Politèctnica de Catalunya, Barcelona, Spain
[d] IEEC Institut d'Estudis Espacials de Catalunya, Barcelona, Spain

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ABSTRACT

The residual accelerations that are typically present in microgravity environments (g-jitters) contain a broad spectrum of frequencies and may be modeled as stochastic processes. Their effects on the quality of the semiconductor crystals are analyzed here quantitatively with direct numerical simulation. In particular we focus on the dopant segregation effects due to thermosolutal convection as a function of the parameters characterizing the statistics of the stochastic force. The numerical simulation is specified for material parameters of two doped semiconductors (Ge:Ga and GaAs:Se) in realistic conditions of actual microgravity environments. As a general result, we show that the segregation response is strongly dominated by the low-frequency part of the g-jitter spectrum. In addition, we develop a simplified model of the problem based on linear response theory that projects the dynamics into very few effective modes. 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.

1. Introduction

The impact of different mechanical disturbances on crystal quality is a longstanding and crucial issue in crystal growth under microgravity conditions [1–5]. Typical disturbances in microgravity environments involve different accelerations in the form of quasi-steady residual values, short pulses, pulse trains of finite duration and high frequency background signals or g-jitters [6–12]. Since the frequency structure of realistic accelerometric signals is often very complex due to the large number of uncontrolled sources that may be present in a given microgravity environment, a possible strategy that has been proposed is to model g-jitters as stochastic processes, in particular because it is difficult to assess a priori the extent to which the linear superposition principle of the effects of the forcing at different frequencies can be invoked in general, due to nonlinearities of the equations.

Stochastic characterization of real g-jitters was first discussed in Ref. [13], and stochastic modeling of g-jitters was applied to different physical processes relevant to both fundamental physics and space technology, such as in coarsening of colloidal suspensions [13], fluid-fluid interfaces [14,15] and in thermal natural convection [16]. In the present paper we pursue this approach in a realistic modelization of different prototypic setups of crystal growth in microgravity in the context of semiconductor materials. As impact indicators we use here the time evolution of the longitudinal and transversal segregation parameters. Following Refs. [14–16], we will model a generic stochastic acceleration environment by means of the so-called narrow-band noise, a rather general Gaussian stochastic process that is characterized by three parameters: the noise intensity, a characteristic dominant frequency where it may be peaked, and a correlation time that controls band width of the frequency spectrum. This stochastic process interpolates between the two extreme cases of white noise and single-frequency noise.

The convective response of the velocity field in a cavity with a stochastic g-jitter transversal to a thermal gradient in a generic fluid configuration was studied in detail in [16]. Here we will extend that approach to include typical confined crystal growth configurations and the coupling of the dopant concentration field to the flow field. We will also focus on parameter values and configurations that are as close as possible to realistic conditions of actual solidification setups in space. Therefore, we aim at a

* Corresponding author at: Departament de Química Física i Inorgìnica, Universitat Rovira i Virgili, Tarragona, Spain.
E-mail address: josepxavier.ruiz@urv.cat (X. Ruiz).

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quantitative characterization of segregation phenomena as a function of the statistics of the g-jitter. Furthermore, we will propose a simplified heuristic model that captures the behavior of the system with a remarkable accuracy with only a few parameters to be obtained from the full integration once and for all. The model provides a qualitative and quantitative understanding of the response of the dopant field to the acceleration driving forces, and becomes a predictive tool to check the effects of any arbitrary acceleration signal with a considerably reduced numerical effort. As a general conclusion, we will find that the system response is strongly dominated by the low-frequency components of the forcing.

2. Definition of the model and numerical integration

2.1. The problem: setup and physical context

We study the directional solidification of a semiconductor melt inside an ampoule with a dopant as a diluted solute and in the presence of a weak fluctuating gravity. See Fig. 1 for a sketch of the geometrical configuration used. The density gradients that drive natural convection receive in general contributions from both temperature and solute concentration fields. However, in the case of the present semiconductors, the dopant concentration is sufficiently small to neglect its contribution to buoyancy when compared to that due to thermal expansion. In addition, the typically small Prandtl numbers of both semiconductors imply that thermal field is only weakly affected by the induced convection and in general it reaches its essentially steady configuration in a very short transient. On the other hand, the solute diffusion is slower. Solute is expelled by the advancement of the solidification front, which forms a layer ahead the interface. This solute layer, in the absence of gravity, has a width of the order of the diffusion length D/v_p and, as shown by Tiller et al. [17], is built on a time scale of the order of D/kv_p^2, D being the solute diffusivity, k being the segregation coefficient and v_p being the velocity of the solidification front imposed externally (see also Refs. [18–20]).

Due to the incompressibility of the liquid phase, any residual acceleration can be assimilated to an effective (time-dependent) gravity, which will in general induce some degree of convection due to thermal buoyancy. Accordingly, there will be a significant solutal transport due to advection that will in general result in an inhomogeneous concentration profile in the final crystal. Our objective in this study is to correlate the type of time dependent residual gravity to the dopant segregation resulting from the thermally induced solutal convection.

Within a perturbative approach of the effect of the residual gravity, it makes sense to consider only an effective gravity vector that is oriented transversally to the advance of the solidification front. This is due to the fact that only the components of the density gradient that are perpendicular to the effective gravity do generate vorticity in the flow, and to lowest order the density gradient is oriented longitudinally. Transversal components of the density gradient will only be generated by convection due to the residual gravity and therefore their coupling to possible longitudinal components of gravity would correspond to higher order corrections. The geometric arrangement is thus that of natural (lateral) convection. Note that components of gravity parallel to the main density gradient can in principle generate convection through a Rayleigh–Bénard instability, but this would only occur for much larger values of gravity. We will also assume that the effective gravity has zero mean. If the mean value is significantly different from zero, then the nature of the problem is fundamentally different as it will be dominated by this constant component.

In our simulations we switch on the time dependence of the residual gravity at a time when the solidification length is roughly 25% of the total length, so that the density profile has already developed when g-jitter starts. This is done for simplicity in order to avoid nontrivial and nongeneric effects associated with the

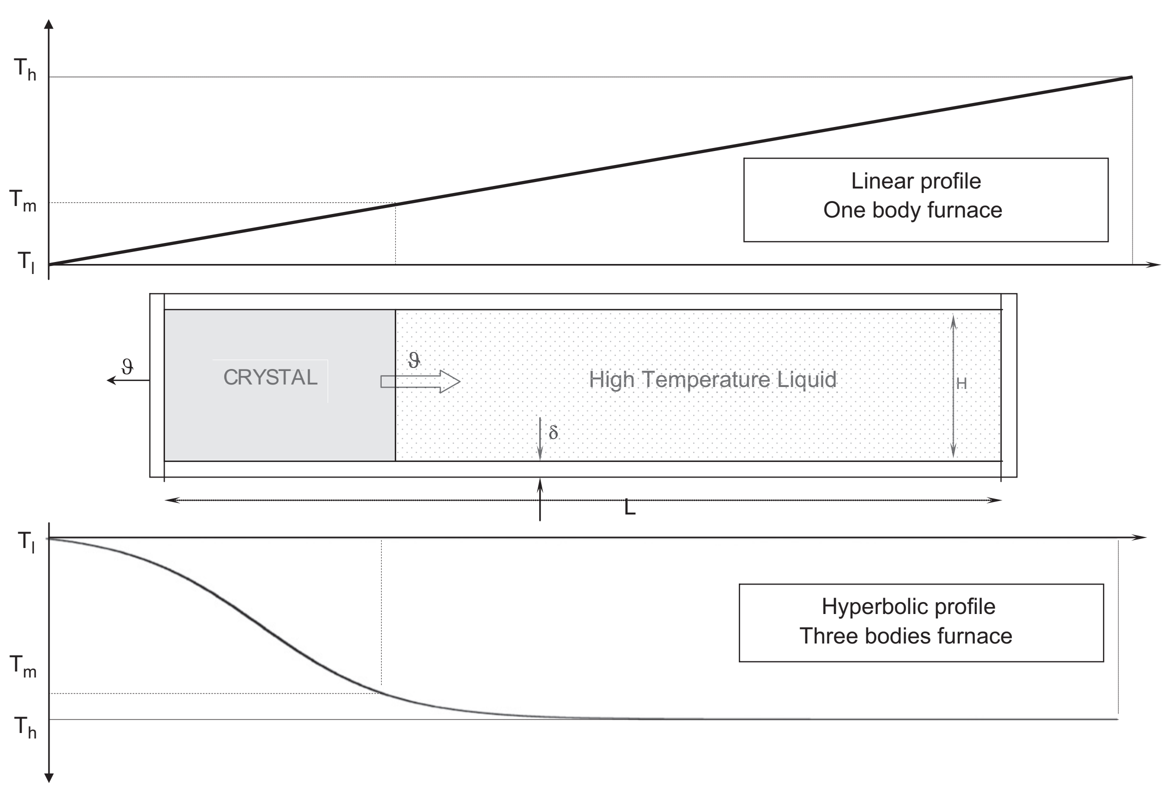

Fig. 1. Global setup of the problem. Top and bottom: sketches of the two thermal profiles employed in the work (see text).