

Analyses of Effects of Residual Accelerations and g-jitter on Semiconductor Melts

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Buoyancy convection induced in a semiconductor solution by gravity fluctuations is studied numerically. Buoyancy forces based on the temperature and concentration differences are taken into account. The residual gravity is 0 g and 10^{-4} g and the amplitude of gravity fluctuation is 10^{-4} g and 10^{-3} g. The frequency of gravity fluctuation is changed from 10^{-3} Hz to 10 Hz. The effect of the amplitude and frequency of gravity fluctuation on the velocity, temperature and concentration fields is investigated and the bifurcation diagrams are produced. Through this analysis, the following results were obtained; (1) The amplitudes of velocity, temperature and concentration fluctuations are small when the frequency of gravity fluctuation is high but they become large when the frequency of gravity fluctuation is lower than 0.01 Hz. (2) The fluctuations of velocity, temperature and concentration deviate from sinusoidal curves and bifurcations occur as the frequency of gravity fluctuation decreases. (3) The amplitude of concentration fluctuations becomes smaller under residual gravity than in the absence of residual gravity.

1. Introduction

One of the factors which determine the quality of grown crystal is convective instabilities induced in melt or solution during the crystal growth process. Therefore, microgravity experiments of crystal growth have been intensively carried out using microgravity experimental facilities in recent years in order to reduce buoyancy convection and grow high quality crystals [1],[2]. However, striations have still been created even in space grown crystals [2],[3]. One possible cause of such nonuniform crystals is Marangoni convection induced in melt or solution during crystal growth processes, which cannot be reduced even under microgravity conditions. Marangoni convection may cause constitutional supercooling in the solution and time-dependent Marangoni convection may induce compositional nonuniformity in grown crystals. Therefore, the onset of oscillatory Marangoni instabilities and the oscillatory mode have been studied theoretically,

numerically and experimentally [4]-[12]. Another cause of nonuniform crystal production may be gravity fluctuations which are called g-jitters. g-jitters are induced in microgravity experimental facilities such as rockets, satellites or space stations. The amplitudes and frequencies of g-jitters have been measured in rockets by Hamacher *et al* [13],[14]. The amplitude of g-jitters is of the order of 10^{-4} g or 10^{-3} g and the frequency varies from 10^{-3} to 10^2 Hz. Convective instabilities induced by g-jitters have also been studied theoretically and numerically [15]-[22]. However, linear analyses have been mainly carried out assuming that the amplitudes of g-jitters are not large enough to induce nonlinear instabilities. Probably this assumption is correct in the case of melt growth of semiconductors or metals since the Prandtl number is as small as 0.01 and therefore the temperature field is not seriously deformed. But this assumption may not apply in the case of solution growth. Although the Prandtl number is very small,

the Schmidt number is quite large because the diffusion coefficient of solute atoms is rather small (usually the order of the diffusion coefficient is 10^{-9} or $10^{-8} \text{ m}^2\text{s}^{-1}$).

In this paper, nonlinear convection induced in a semiconductor solution by g-jitters is analysed numerically and the effect of the residual gravity and the amplitude and frequency of g-jitters on the velocity, temperature and concentration fields is investigated. In the second section, a numerical modelling and technique are described. In the third section, the results of the calculations are shown and nonlinear instabilities induced by g-jitters are investigated and discussed. In the final section, the results of the numerical analyses are summarised.

2. Numerical modelling and procedure

The calculation model is shown in Figure 1. A binary solution is confined in a two-dimensional square container. The left wall is heated and the right wall is cooled. The top and bottom walls are thermally insulated. The concentrations at the left and right walls are fixed. The concentration at the left wall is higher than that at the right wall and there is no mass transfer through the top and bottom walls. The gravity acts in the $-Z$ direction. The residual gravity is 0 g and 10^{-4} g and the amplitude of gravity

fluctuation is 10^{-4} g and 10^{-3} g . The responses of convection to sinusoidal gravity fluctuations are investigated changing the frequency from 10^{-3} to 10 Hz .

The coordinate r , time t , pressure p , velocity v , temperature T and concentration c being nondimensionalised as equation(1), the nondimensional governing equations are introduced as equations (2)-(5).

$$\begin{aligned} R &\equiv \frac{r}{L}, \quad \tau \equiv \frac{t}{L^2/\nu}, \\ P &\equiv \frac{p}{\rho\nu^2/L^2}, \quad V \equiv \frac{v}{\nu/L}, \\ \theta &\equiv \frac{T - T_0}{T_1 - T_0}, \quad C \equiv \frac{c - c_0}{c_1 - c_0} \end{aligned} \quad (1)$$

where L , ν and ρ are, respectively, the depth of the solution layer, the kinetic viscosity and the density. T_1 , T_0 and c_1 , c_0 are, respectively, temperature and concentration at the left and right walls.

Continuity equation

$$\text{div } V = 0 \quad (2)$$

Momentum equation

$$\begin{aligned} \frac{\partial V}{\partial \tau} + (V \text{grad})V &= -\text{grad}P + \Delta V \\ &+ \frac{1}{Pr} (Ra^T + Ra_j^T \sin \Omega \tau) \theta \cdot e \\ &+ \frac{1}{Sc} (Ra^C + Ra_j^C \sin \Omega \tau) C \cdot e \end{aligned} \quad (3)$$

where e is the unit vector in the Z direction.

Temperature transport equation

$$\frac{\partial \theta}{\partial \tau} + (V \text{grad})\theta = \frac{1}{Pr} \Delta \theta \quad (4)$$

Concentration transport equation

$$\frac{\partial C}{\partial \tau} + (V \text{grad})C = \frac{1}{Sc} \Delta C \quad (5)$$

Ra^T , Ra_j^T , Ra^C , Ra_j^C , Ω , Pr and Sc are, respectively,

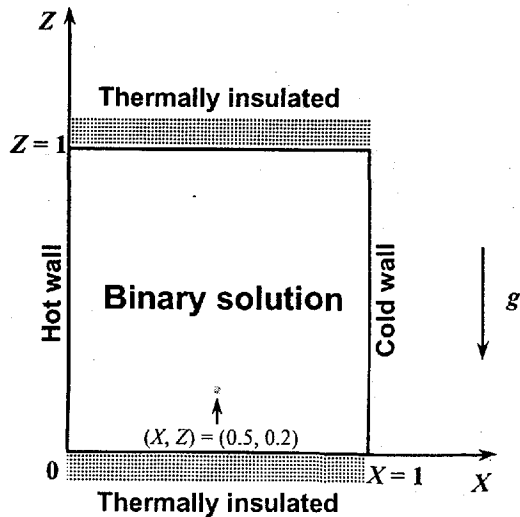


Figure 1 Calculation model of convective instability

the Rayleigh number based on the temperature difference and residual gravity, the Rayleigh number based on the temperature difference and g-jitter, the Rayleigh number based on the concentration difference and residual gravity, the Rayleigh number based on the concentration difference and g-jitter, the nondimensional angular frequency of g-jitter, the Prandtl number and the Schmidt number, which are summarised below.

$$\begin{aligned} Ra^T &\equiv \frac{\beta g \Delta T L^3}{\kappa \nu}, & Ra_j^T &\equiv \frac{\beta g_A \Delta T L^3}{\kappa \nu} \\ Ra^C &\equiv \frac{\gamma g \Delta c L^3}{D \nu}, & Ra_j^C &\equiv \frac{\gamma g_A \Delta c L^3}{D \nu} \\ Pr &\equiv \frac{\nu}{\kappa}, & Sc &\equiv \frac{\nu}{D}, & \Omega &\equiv \frac{2\pi f}{\nu/L^2} \end{aligned} \quad (6)$$

where β , κ , γ , D , ΔT , Δc , f , and g_A are, respectively, the temperature coefficient of volume expansion, the thermal diffusivity, the concentration coefficient of volume expansion, the diffusion coefficient, the temperature difference between the left and right walls, the concentration difference between the left and right walls, the frequency of g-jitter and the amplitude of g-jitter.

The boundary conditions are listed below.

$$\begin{aligned} X = 0; & \quad V_X = 0, V_Z = 0, \Psi = 0, \\ & \quad \theta = 1, C = 1 \\ X = 1; & \quad V_X = 0, V_Z = 0, \Psi = 0, \\ & \quad \theta = 0, C = 0 \\ Z = 0; & \quad V_X = 0, V_Z = 0, \Psi = 0, \\ & \quad \frac{\partial \theta}{\partial Z} = 0, \frac{\partial C}{\partial Z} = 0 \\ Z = 1; & \quad V_X = 0, V_Z = 0, \Psi = 0, \\ & \quad \frac{\partial \theta}{\partial Z} = 0, \frac{\partial C}{\partial Z} = 0 \end{aligned} \quad (7)$$

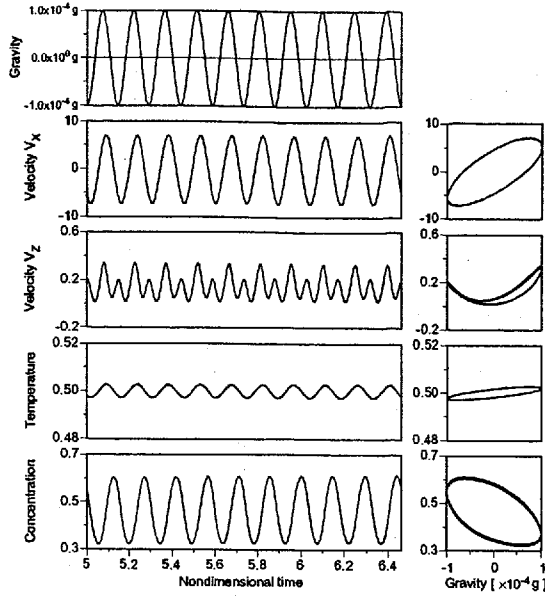
The values of the nondimensional parameters shown in equation(6) were estimated based on the physical properties of GaAs [23]-[25]. The Prandtl number and the Schmidt number are 0.01 and 15, respectively. We set the temperature difference between the walls and the depth of the solution at

100 K and 10^{-2} m, respectively. In this case, the Rayleigh numbers Ra^T and Ra^C are, respectively, 11 and 2.1×10^4 when the residual gravity is 10^{-4} g. The Rayleigh numbers based on g-jitter, Ra_j^T and Ra_j^C , are 11 and 2.1×10^4 when the amplitude of g-jitter is 10^{-4} g and 1.1×10^2 and 2.1×10^5 when the amplitude of g-jitter is 10^{-3} g.

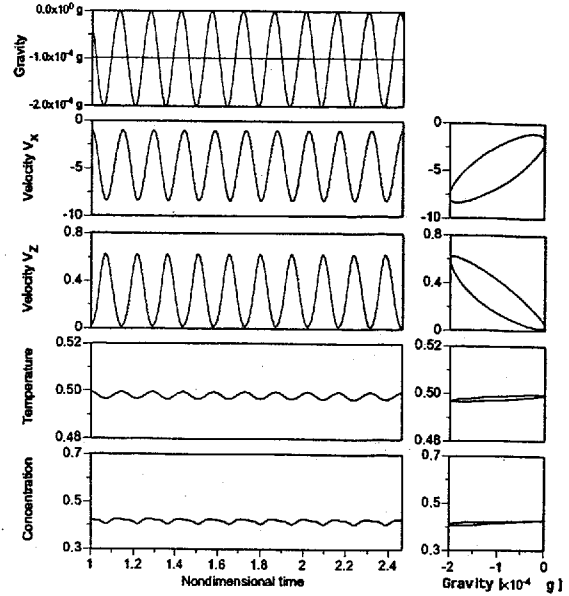
As two-dimensional analysis is carried out in this study, we introduced the stream function and vorticity. We solved equations(2)-(5) under the boundary conditions (7) by the finite difference method. The time derivatives are approximated by the first-order explicit formula and the nonlinear convection terms are approximated by the fourth-order central difference formula. The other spatial derivatives are approximated by the second-order central difference formula. The vorticity equation was solved by the SOR method [26]. The number of grids in the calculation space was changed such as 21×21 , 41×41 and 61×61 and the maximum difference in the stream functions, vorticities, temperatures and concentrations caused by the grid number differences was within 5 %.

3. Result and discussion

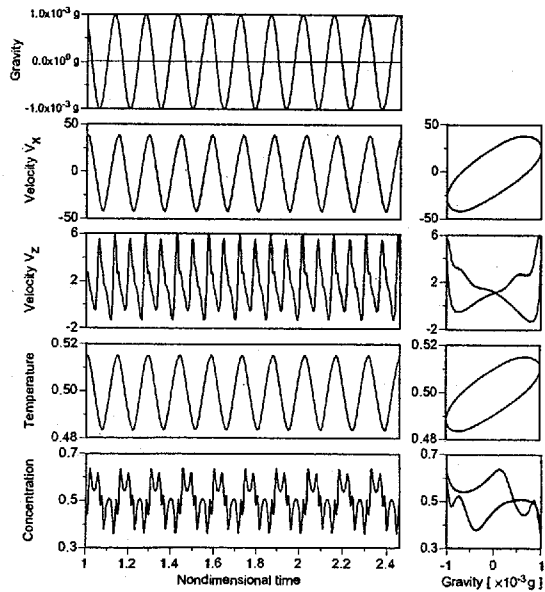
The calculation was successfully carried out without any numerical instabilities. The time variations of the velocities V_x , V_z , temperature and concentration at $(X, Z) = (0.5, 0.2)$ are shown in Figure 2 where the residual gravity is 0 g and 10^{-4} g, the amplitude of g-jitter is 10^{-4} g and 10^{-3} g and the frequency of g-jitter is 0.01 Hz. The cross-correlations between the fluctuations of velocities, temperature and concentration and the gravity fluctuation are also shown in Figure 2. When the frequency of g-jitter is higher than 0.1 Hz, the fluctuations of velocities, temperature and concentration are sinusoidal, whereas the fluctuations become deformed showing bifurcations as the frequency of g-jitter decreases. As the Prandtl number is as small as 0.01, the temperature field is not deformed seriously. On the other hand, the concentration field is very sensitive to g-jitters and deformed greatly since the Schmidt number is large and therefore the nonlinear effect becomes dominant.



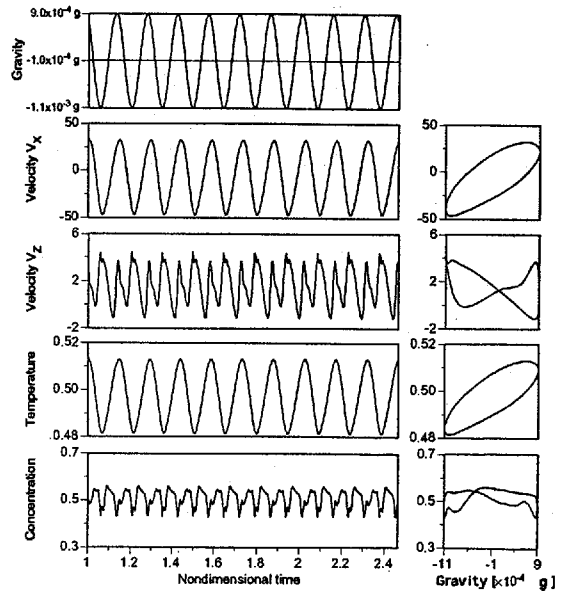
(a) The residual gravity is 0 g and the amplitude of g-jitter is 10^{-4} g.



(c) The residual gravity is 10^{-4} g and the amplitude of g-jitter is 10^{-4} g.



(b) The residual gravity is 0 g and the amplitude of g-jitter is 10^{-3} g.



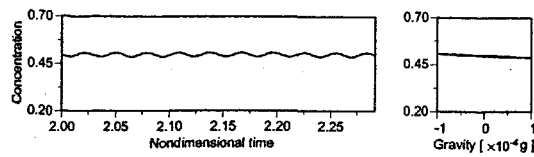
(d) The residual gravity is 10^{-4} g and the amplitude of g-jitter is 10^{-3} g.

Figure 2 Time variations of gravity, velocities V_x , V_z , temperature and concentration
The frequency of g-jitter is 0.01.

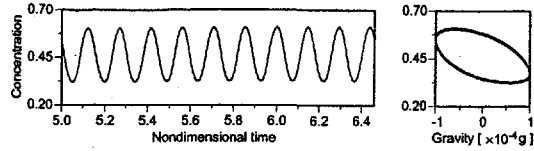
The amplitude of concentration fluctuation becomes larger in the absence of residual gravity than under residual gravity.

The time variations of concentration at $(X, Z) = (0.5, 0.2)$ are shown in Figure 3 where the residual gravity is 0 g and 10^{-4} g and the amplitude of g-jitter

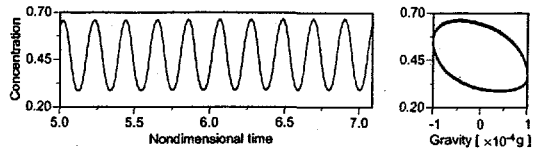
is 10^{-4} g and 10^{-3} g. The cross-correlations between the concentration fluctuation and the gravity fluctuation are also shown in Figure 3. As we mentioned above, the residual gravity reduces the amplitude of the concentration fluctuation and the concentration fluctuation becomes more complicated



(i) The frequency of gravity fluctuation is 0.05 Hz

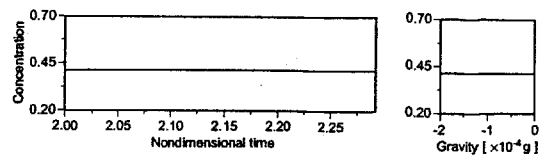


(ii) 0.01 Hz

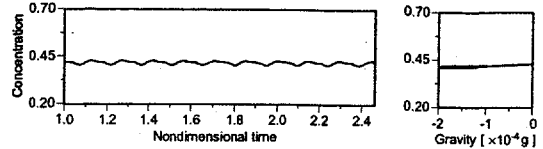


(iii) 0.007 Hz

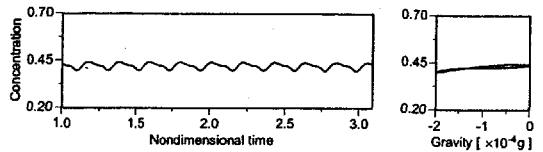
(a) The residual gravity is 0 g and the amplitude of g-jitter is 10^{-4} g.



(i) The frequency of gravity fluctuation is 0.05 Hz

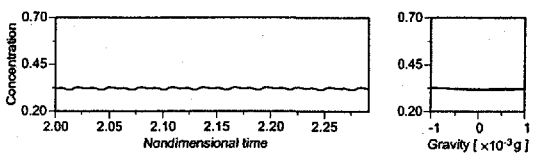


(ii) 0.01 Hz

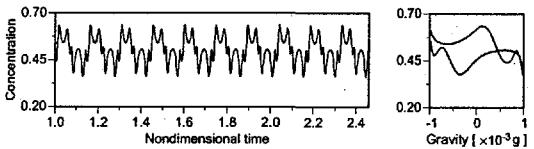


(iii) 0.007 Hz

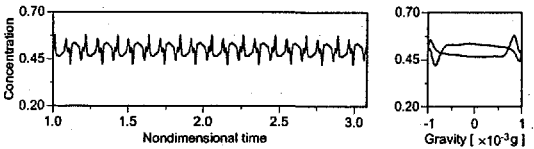
(c) The residual gravity is 10^{-4} g and the amplitude of g-jitter is 10^{-4} g.



(i) The frequency of gravity fluctuation is 0.05 Hz

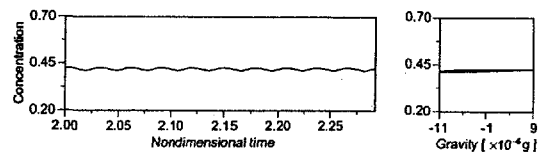


(ii) 0.01 Hz

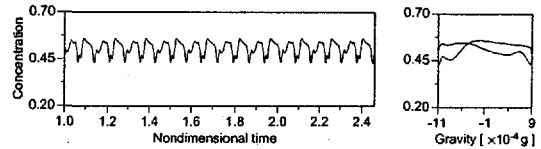


(iii) 0.007 Hz

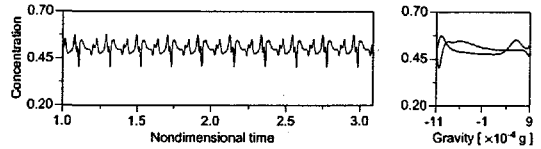
(b) The residual gravity is 0 g and the amplitude of g-jitter is 10^{-3} g.



(i) The frequency of gravity fluctuation is 0.05 Hz



(ii) 0.01 Hz



(iii) 0.007 Hz

(d) The residual gravity is 10^{-4} g and the amplitude of g-jitter is 10^{-3} g.

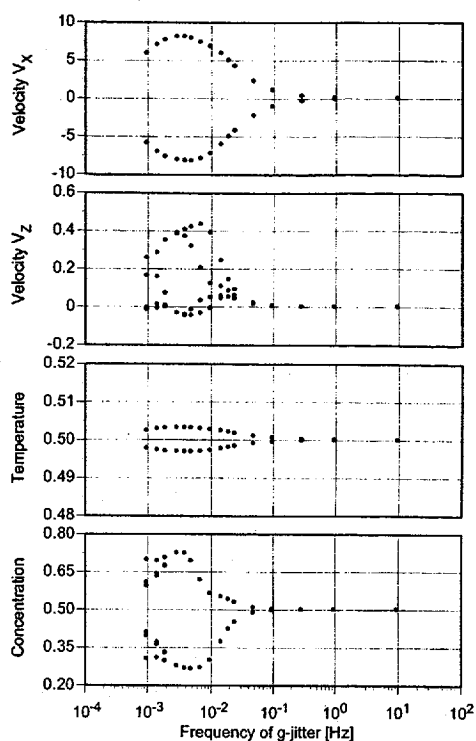
Figure 3 Time variations of concentration

showing bifurcations as the frequency of g-jitter decreases and the amplitude of g-jitter increases.

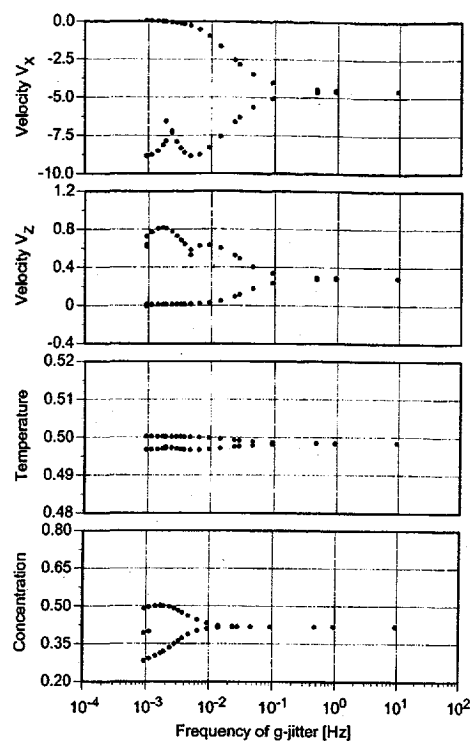
The bifurcation diagrams of the velocity, temperature and concentration fluctuations are shown in Figure 4. When the frequency of g-jitter is higher than 0.1 Hz, the amplitudes of the velocity, temperature and concentration fluctuations are small

and the fluctuations are sinusoidal. Bifurcations appear with a decrease in the frequency of g-jitter. The nonlinear effect becomes dominant even when the amplitude of g-jitter is as small as 10^{-4} g or 10^{-3} g if the frequency of gravity fluctuation is lower than 0.01 Hz.

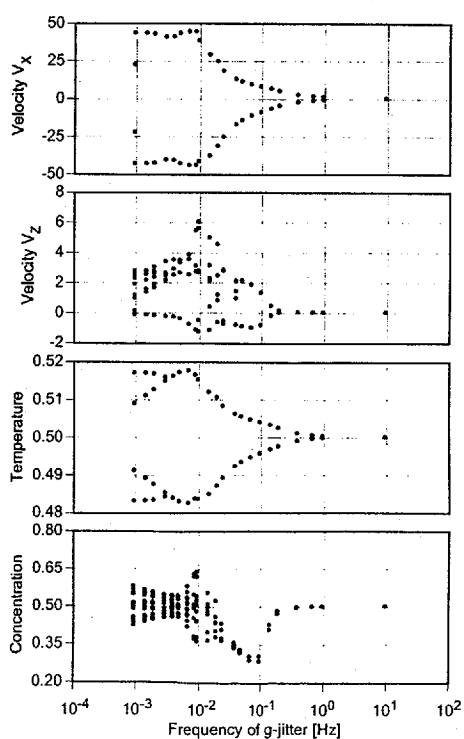
G-jitters may not become a serious problem in



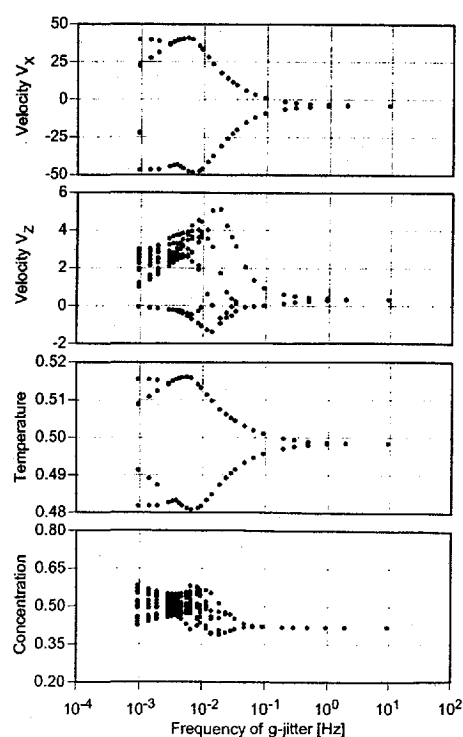
(a) The residual gravity is 0 g and the amplitude of g-jitter is 10^{-4} g.



(c) The residual gravity is 10^{-4} g and the amplitude of g-jitter is 10^{-4} g.



(b) The residual gravity is 0 g and the amplitude of g-jitter is 10^{-3} g.



(d) The residual gravity is 10^{-4} g and the amplitude of g-jitter is 10^{-3} g.

Figure 4 Bifurcation diagrams of velocity, temperature and concentration

the case of melt growth of semiconductors or metals since the Prandtl number is very small. The temperature field is not seriously deformed and the amplitude of temperature fluctuation is small in this case. However, g-jitters may affect the quality of semiconductors grown by the solution growth technique because the Schmidt number is large. Especially, when the frequency of g-jitter is low, the concentration fluctuations become very complicated. Although residual gravity reduces the amplitude of concentration fluctuation, it also causes constitutional supercooling [27] and, therefore, is undesirable. Therefore, an intelligent method of reducing low frequency gravity fluctuations and residual gravity must be found or invented for future crystal growth in space. A digital control system is proposed to reduce the amplitude of g-jitters [28] but the authors concluded that reducing low frequency g-jitters was very difficult. The application of a magnetic field may be another way of reducing concentration fluctuations. Definitely fluctuations are reduced in a dc magnetic field [29]-[31], but this may not prove a viable option from a practical point of view as the intensity of magnetic field must be very high. It seems that applying an ac magnetic field is more effective [32]. We need further investigations of the magnetohydrodynamic effect on the suppression of time-dependent instabilities induced by low frequency g-jitters.

4. Conclusion

We analysed velocity, temperature and concentration fluctuations induced by g-jitters in a semiconductor solution. The nonlinear heat and mass transfer equations were solved numerically. The calculations were successfully carried out and the following results were obtained; (1) The amplitudes of velocity, temperature and concentration fluctuations are small when the frequency of gravity fluctuation is high but they become large when the frequency of gravity fluctuation is lower than 0.01 Hz. (2) The fluctuations of velocity, temperature and concentration deviate from sinusoidal curves and bifurcations occur as the frequency of gravity fluctuation decreases. (3) The amplitude of

concentration is reduced by residual gravity.

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