

Theoretical gravity studies on roles of convection in crystal growth of $\text{Hg}_2\text{Cl}_2\text{-Xe}$ by physical vapor transport under normal and high gravity environments

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Abstract Particular interest in the role of convection in vapor crystal growth has arisen since some single crystals under high gravity acceleration of $10g_0$ appear considerably larger than those under normal gravity acceleration ($1g_0$). For both $\Delta T = 60$ K and 90 K, the mass flux increases by a factor of 3 with increasing the gravity acceleration from $1g_0$ up to $10g_0$. On the other hand, for $\Delta T = 30$ K, the flux is increased by a factor of 1.36 for the range of $1g_0 \leq g \leq 10g_0$. The maximum growth rates for $1g_0$, $4g_0$, $10g_0$ appear approximately in the neighborhood of $y = 0.5$, and the growth rates shows asymmetrical patterns, which indicate the occurrence of either one single or more than one convective cell. The maximum growth rate for $10g_0$ is nearly greater than that for $1g_0$ by a factor of 2.0 at $P_B = 20$ Torr. For three different gravity levels of $1g_0$, $4g_0$ and $10g_0$, the maximum growth rates are greater than the minimum rates by a factor of nearly 3.0, based on $P_B = 20$ Torr. The mass flux increases with increasing the gravity acceleration, for $1g_0 \leq g_y \leq 10g_0$, and decreases with increasing the partial pressure of component B, xenon (Xe), P_B . The $|U|_{\max}$ is directly proportional to the gravity acceleration for $20 \text{ Torr} \leq P_B \leq 300 \text{ Torr}$. As the partial pressure of P_B (Torr) decreases from 300 Torr to 20 Torr, the slopes of the $|U|_{\max}$ s versus the gravity accelerations increase from 0.1 sec to 0.17 sec. The mass flux of Hg_2Cl_2 is exponentially decayed with increasing the partial pressure of component B, P_B (Torr) from 20 Torr up to 300 Torr.

Key words Mercurous chloride, Convection, Xenon, gravity, Physical vapor transport

1. Introduction

Physical vapor transport (PVT) has become an important crystal growth process for a variety of acousto-optic materials. The mechanism of the PVT process is simple: sublimation-condensation in closed silica glass ampoules in temperature gradient imposed between the source material and the growing crystal. It also requires minimal process control and monitoring, and transport results are easily interpreted. Of particular importance is the use of PVT for materials processing experiments in low and high gravity environments, which would provide a better and thorough understanding of transport phenomena occurring in the vapor phase and crystal growth phenomena.

Over the past 25 years many theoretical modeling studies [1-12] on transport phenomena in PVT and much quantitative experiments [13-20] have been extensively investigated. Most important theoretical works were achieved by Rosenberger [1-4, 6, 8] and, recently

extended for transition to chaos flow fields in specialty materials of mercurous chloride in applications of microgravity experiments by Duval [21-25]. They have addressed the underlying phenomena in the PVT processes on the relative importance and influencing parameters of diffusion-advection, thermal and/or solutal convection on mass transport. Our recent studies [26-33] are for PVT processes of specialty materials such as mercurous halides (Hg_2Cl_2 and Hg_2Br_2) under normal and microgravity environments to investigate the role of convection on the mass transport rate and its transition from diffusion-dominated to circulatory convection-dominated regimes in relation to total pressure, temperatures of source and crystal ends, aspect ratio (transport length-to-width), molecular weights, wall temperature profiles.

It is the purpose of this paper to study systematically the transport phenomena covering the various gravity accelerations in the PVT processes of Hg_2Cl_2 crystal growth system. For this theoretical analysis of the PVT processes, a two-dimensional model is in horizontally oriented, cylindrical, closed ampoules in a two-zone furnace system. Diffusion-limited processes are considered in this paper, although Singh, Mazelsky and Glicksman [34] demonstrated that the interface kinetics plays an important

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role in the PVT system of Hg_2Cl_2 . The effects of normal and high gravity accelerations on solutally and/or thermally buoyancy-driven convection will be considered at this point, primarily for a mixture of Hg_2Cl_2 vapor and impurity of Xenon (Xe), although for gaining insights into the convection, the low gravity environments are more important than high gravity conditions in some cases.

2. The Model

Mercurous chloride (Hg_2Cl_2) materials are important for applications in acousto-optic and opto-electronic devices such as Bragg cells, X-ray detectors operating at ambient temperature [35]. The equimolar Hg_2Cl_2 compound decomposes to two liquids at a temperature near 525°C where the vapor pressure is above 20 atm [36, 37]. Because of this decomposition and high vapor pressure, Hg_2Cl_2 cannot be solidified as a single crystal directly from the stoichiometric melt. However, very similar to the mercurous bromide, mercurous chloride exhibits sufficiently high vapor pressure at low temperatures so that these crystals are usually grown by the physical vapor transport (PVT) in closed silica glass ampoules.

Consider a rectangular enclosure of height H and transport length L , shown in Fig. 1. The source is maintained at a temperature T_s , while the growing crystal is at a temperature T_c , with $T_s > T_c$. PVT of the transported component A (Hg_2Cl_2) occurs inevitably, due to presence of impurities, with the presence of a component B (Xe). The interfaces are assumed to be flat for simplicity. The finite normal velocities at the interfaces can be expressed by Stefan flow deduced from the one-dimensional diffusion-limited model [38], which would provide the coupling between the fluid dynamics and species calculations. On the other hand, the tangential

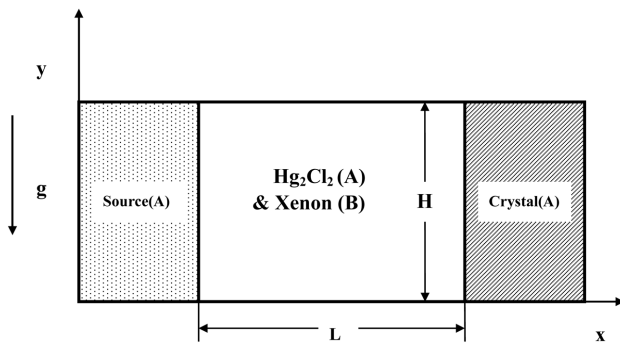


Fig. 1. Schematic and coordinates for a PVT crystal growth reactor of Hg_2Cl_2 -Xe in a two-dimensional rectangular system.

component of the mass average velocity of the vapor at the interfaces vanishes. Thermodynamic equilibria are assumed at the interfaces so that the mass fractions at the interfaces are kept constant at $\omega_{A,s}$ and $\omega_{A,c}$. On the vertical non-reacting walls appropriate velocity boundary conditions are no-slip, the normal concentration gradients are zero, and wall temperatures are imposed as nonlinear temperature gradients. Thermo-physical properties of the fluid are assumed to be constant, except for the density. When the Boussinesq approximation is invoked, density is assumed constant except the buoyancy body force term. The density is assumed to be a function of both temperature and concentration. The ideal gas law and Dalton's law of partial pressures are used. Viscous energy dissipation and the Soret-Dufour (thermo-diffusion) effects can be neglected, as their contributions remain relatively insignificant for the conditions encountered in our PVT crystal growth processes. The transport of fluid within a rectangular PVT crystal growth reactor is governed by a system of elliptic, coupled conservation equations for mass (continuity), momentum, energy and species (diffusion) can be represented by the generic Eq. (1) [39] with their appropriate boundary conditions Eqs. (2) through (4). Let u_x, u_y denote the velocity components along the x - and y -coordinates in the x, y rectangular coordinate, and let T, ω_A, p denote the temperature, mass fraction of species A (Hg_2Cl_2) and pressure, respectively, where the superscript of $*$ denotes the dimensionless [26-33].

$$\nabla \bullet (\rho u \phi) = \nabla \bullet (\Gamma \nabla \phi) + S, \quad (1)$$

On the walls ($0 < x^* < L/H, y^* = 0$ and 1):

$$u^*(x^*, 0) = u^*(x^*, 1) = v^*(x^*, 0) = v^*(x^*, 1) = 0 \quad (2)$$

$$\frac{\partial \omega_A^*(x^*, 0)}{\partial y^*} = \frac{\partial \omega_A^*(x^*, 1)}{\partial y^*} = 0,$$

$$T^*(x^*, 0) = T^*(x^*, 1) = \frac{T - T_c}{T_s - T_c}$$

On the source ($x^* = 0, 0 < y^* < 1$):

$$u^*(0, y^*) = -\frac{1}{\text{Le}(1 - \omega_{A,s})} \frac{\partial \omega_A^*(0, y^*)}{\partial x^*}, \quad (3)$$

$$v^*(0, y^*) = 0,$$

$$T^*(0, y^*) = 1,$$

$$\omega_A^*(0, y^*) = 1.$$

On the crystal ($x^* = L/H, 0 < y^* < 1$):

$$u^*(L/H, y^*) = -\frac{1}{\text{Le}(1 - \omega_{A,c})} \frac{\partial \omega_A^*(L/H, y^*)}{\partial x^*}, \quad (4)$$

$$\begin{aligned} v^*(L/H, y^*) &= 0, \\ T^*(L/H, y^*) &= 0, \\ \omega_A^*(L/H, y^*) &= 0. \end{aligned}$$

The vapor pressure [10] p_A of Hg_2Cl_2 (in the unit of Pascal) can be evaluated from the

$$p_A = e^{(a-b/T)}, \quad (5)$$

following formula as a function of temperature: in which $a = 29.75$, $b = 11767.1$.

3. Results and Discussion

The purposes for this study is to correlate the growth rate and the convective intensity to process parameters such as (1) temperature differences between the source and the crystal region, (2) partial pressures of component B (Xe), (3) normal and high gravitational levels to investigate the effects of noble inert gas Xe on the convection during physical vapor transport. Thus, it is desirable to express some results in terms of dimensional growth rate, however they are also applicable to parameter ranges over which the process varies in the manner given. The six dimensionless parameters, namely Gr , Ar , Pr , Le , C_v and Pe , are independent and arise naturally from the dimensionless governing equations and boundary conditions. The dimensionless parameters and physical properties for the operating conditions of this study are shown in Table 1.

Because the molecular weight of a noble element xenon (Xe) is not equal to that of the crystal component (Hg_2Cl_2) during the physical vapor transport, both

Table 1
Typical thermo-physical properties used in this study ($M_A = 472.086$, $M_B = 131.3$)

Transport length, L	10 cm
Height, H	2 cm
Source temperature, T_s	350°C
Crystal temperature, T_c	260°C
Density, ρ	0.002 g/cm ³
Dynamic viscosity, μ	0.00033 g/(cm · sec)
Diffusivity, D_{AB}	0.36 cm ² /s
Thermal expansion coefficient, β	0.0016 K ⁻¹
Prandtl number, Pr	0.78
Lewis number, Le	0.5
Peclet, Pe	4.13
Concentration number, C_v	1.1
Total system pressure, P_T	413.06 Torr
Partial pressure of component B, P_B	20 Torr
Thermal Grashof number, Gr_t	5.6×10^4
Solutal Grashof number, Gr_s	4.0×10^5

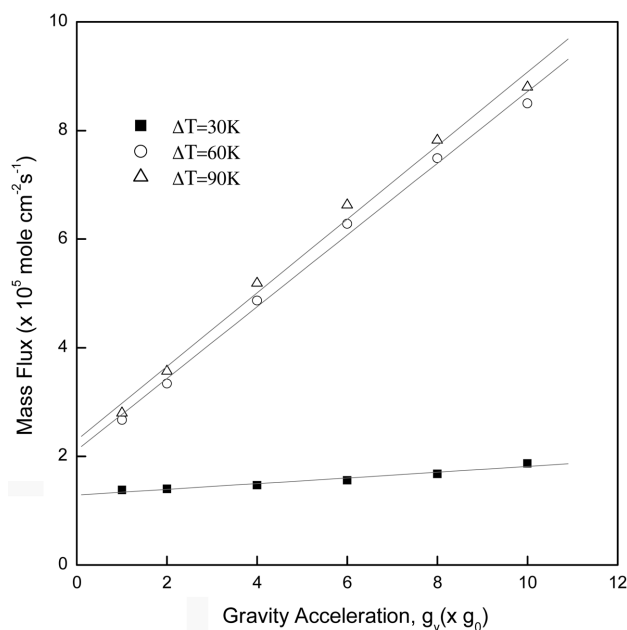


Fig. 2. The mass flux of Hg_2Cl_2 in terms of mole $\text{cm}^{-2}\text{s}^{-1}$ versus gravity acceleration in terms of g_0 (981 cm s^{-2}) for the horizontal orientations for three temperature differences between the source and the crystal regions: $320^\circ\text{C} \rightarrow 290^\circ\text{C}$ (symbol ■), $350^\circ\text{C} \rightarrow 290^\circ\text{C}$ (symbol ○), and $350^\circ\text{C} \rightarrow 260^\circ\text{C}$ (symbol △). Based on $Ar = 5$, $P_B = 20$ Torr, $Ar = 5$, $L = 10$ cm, with the linear temperature profiles at walls.

solutal and/or thermal effects should be considered in this study. The linear temperature profiles at wall boundary conditions only are considered.

Fig. 2 shows the mass flux of Hg_2Cl_2 in terms of mole $\text{cm}^{-2}\text{s}^{-1}$ versus gravity acceleration in terms of g_0 (981 cm s^{-2}) for the horizontal orientations for three temperature differences between the source and the crystal regions: $320^\circ\text{C} \rightarrow 290^\circ\text{C}$ (symbol ■), $350^\circ\text{C} \rightarrow 290^\circ\text{C}$ (symbol ○), and $350^\circ\text{C} \rightarrow 260^\circ\text{C}$ (symbol △). Based on the parameters of $Ar = 5$, $P_B = 20$ Torr, $Ar = 5$, $L = 10$ cm, with the linear temperatures on the walls. For $\Delta T = 90$ K and $g_y = 1g_0$, the governing dimensionless parameters are as follows: aspect ratio $Ar = 5.0$, Prandtl number $Pr = 0.78$, Lewis number $Le = 0.5$, thermal Grashof number $Gr_t = 5.6 \times 10^4$, solutal Grashof number $Gr_s = 4.0 \times 10^5$, Peclet number $Pe = 4.13$, concentration number $C_v = 1.1$. Here, the subscript of 0 denotes the normal gravity acceleration of $981 \text{ cm} \cdot \text{s}^{-2}$. For both $\Delta T = 60$ K and 90 K, the mass flux increases by a factor of 3 with increasing the gravity acceleration from $1g_0$ up to $10g_0$. On the other hand, for $\Delta T = 30$ K, the flux is increased by a factor of 1.36 for the range of $1g_0 \leq g \leq 10g_0$. As shown in Fig. 2, the variation in the flux when increasing the temperature difference from 60 K to up 90 K is insignificant, but important when

increasing from 30 K to 60 K. It is likely to be due to the presence of a sharp increase in total pressure with the corresponding source temperature. In other words, the source temperatures for both $\Delta T = 60$ K and 90 K are 350°C, and 320°C for $\Delta T = 30$ K, respectively. Consequently, under the conditions of gravity accelerations, the mass fluxes for both $\Delta T = 60$ K and 90 K are approximately greater than the flux at $\Delta T = 30$ K by a factor of 2. Although the graph for $T_s = 350^\circ\text{C}$ is not shown here, to prove our inference, comparisons of mass fluxes for $T_s = 320^\circ\text{C}$ and 350°C are made. To be specific, the mass flux at $T_s = 320^\circ\text{C}$ and $1g_0$ is 1.38×10^{-5} mole cm^{-2} s^{-1} ; at $T_s = 350^\circ\text{C}$ and $1g_0$, 2.26×10^{-5} mole cm^{-2} s^{-1} . For $T_s = 350^\circ\text{C}$, the mass flux at $1g_0$ is 1.87×10^{-5} mole cm^{-2} s^{-1} ; at $10g_0$, 6.87×10^{-5} mole cm^{-2} s^{-1} . It is concluded the mass fluxes versus gravity accelerations vary with a relatively similar slope under the condition of same source temperature of 350°C . Note in actual crystal experiments the typical source and crystal temperature correspond to 320°C and 290°C , respectively.

Fig. 3 shows the $|U|_{\text{max}}$ as a function of gravity acceleration for the three temperature differences between the source and the crystal regions, corresponding to Fig. 2. The $|U|_{\text{max}}$ is the dimensional maximum magnitude of the velocity vector, which indicates the intensity of convection in the vapor phase. Fig. 3 illustrates the $|U|_{\text{max}}$ is a direct proportional and linear relationship with the

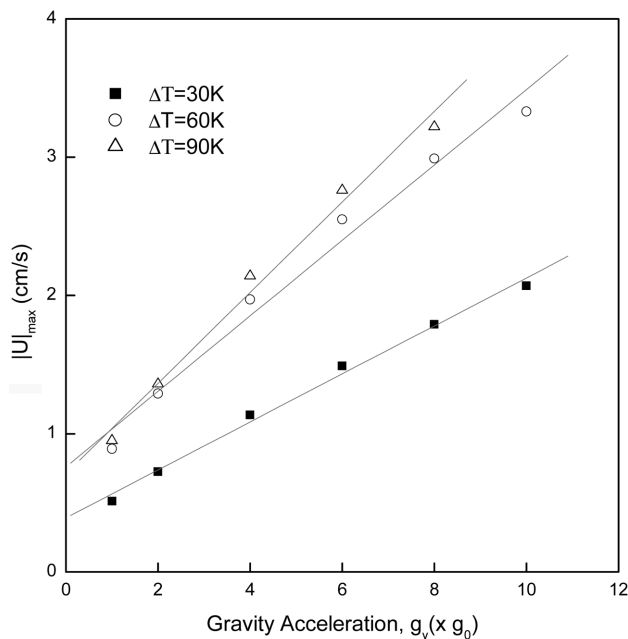


Fig. 3. The $|U|_{\text{max}}$ as a function of gravity acceleration for the three temperature differences between the source and the crystal regions, corresponding to Fig. 2.

gravity acceleration. The three cases of $T = 30$ K, 60 K, and 90 K have a gradient of 0.17, 0.27, and 0.29 $\text{cm s}^{-1} g_0^{-1}$, respectively. The $|U|_{\text{max}}$ is not increased by a factor of 2 as the temperature difference is increased by a factor of 2, but increased by a factor of 1.59 from $\Delta T = 30$ K to 60 K, and after $\Delta T = 60$ K increased by a factor of 1.07 until the temperature difference reaches $\Delta T = 90$ K.

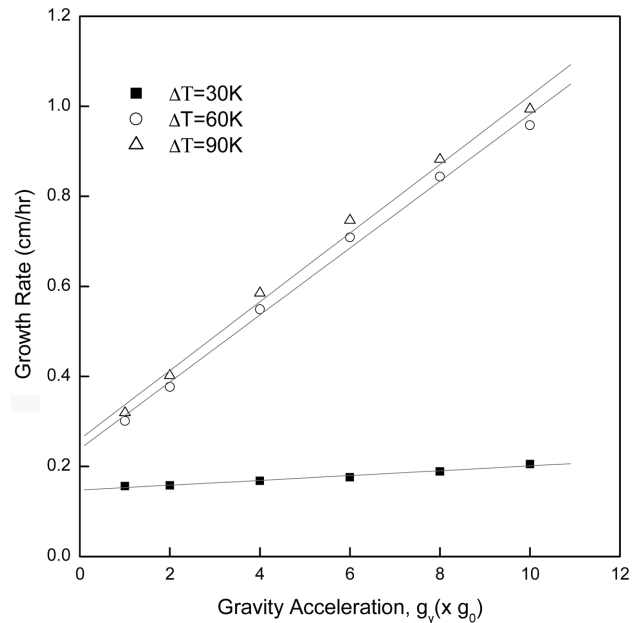


Fig. 4. Relationships between the growth rate and the gravity accelerations for three temperature differences between the source and the crystal regions, corresponding to Fig. 2.

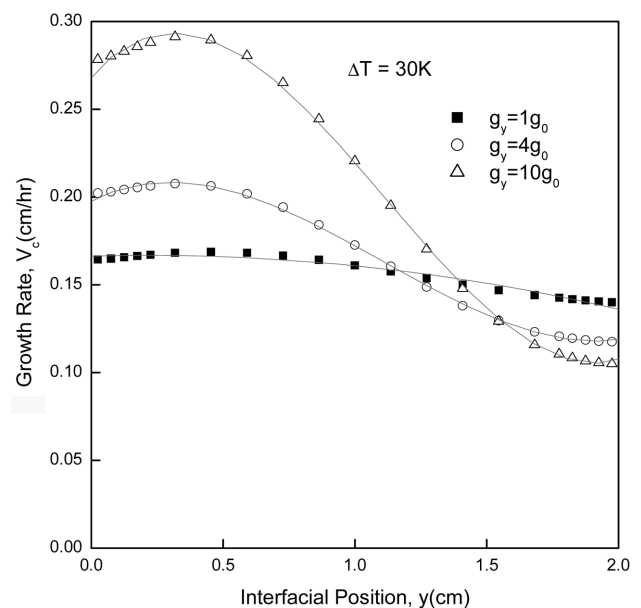


Fig. 5. Interfacial distributions of crystal growth rate of Hg_2Cl_2 for various gravity accelerations, at $\Delta T = 30$ K and $P_B = 20$ Torr. Based on $\text{Ar} = 5.0$, $\text{Pr} = 0.81$, $\text{Le} = 0.34$, $\text{Gr}_t = 8.4 \times 10^3$, $\text{Gr}_s = 9.7 \times 10^4$, $\text{Pe} = 2.38$, $C_v = 1.1$, $g_y = 1g_0$.

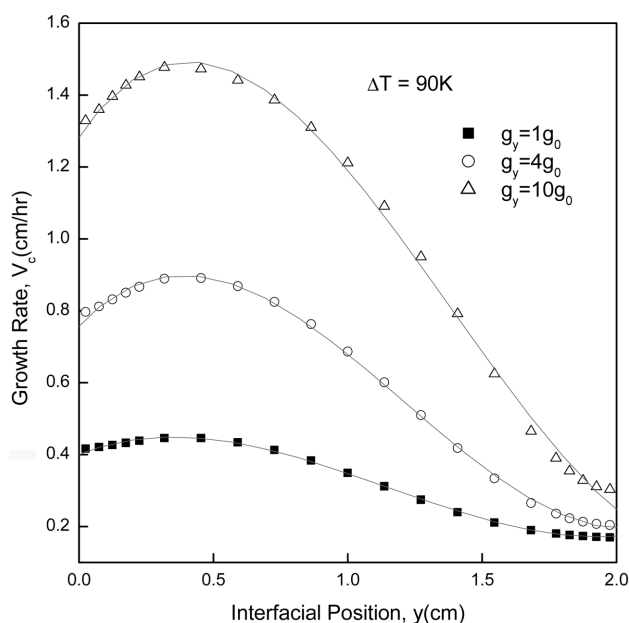


Fig. 6. Interfacial distributions of crystal growth rate of Hg_2Cl_2 for various gravity accelerations, at $\Delta T = 90$ K and $P_B = 20$ Torr. Based on $Ar = 5.0$, $Pr = 0.78$, $Le = 0.5$, $Gr_i = 5.6 \times 10^4$, $Gr_s = 4.0 \times 10^5$, $Pe = 4.13$, $C_v = 1.1$, $g_y = 1g_0$.

Fig. 4 shows the relationships between the growth rate and the gravity accelerations for three temperature differences between the source and the crystal regions, corresponding to Fig. 2. Fig. 4 is prepared from viewpoint of the crystal growth rate (cm/hr) to provide a good frame for Figs. 5 and 6, which show interfacial distributions of crystal growth rate of Hg_2Cl_2 for various gravity accelerations, at $\Delta T = 30$ K and 90 K, respectively. As shown in Fig. 5, the interfacial distributions for three gravity accelerations of $1g_0$, $4g_0$, and $10g_0$ are relatively flat after $y = 1.3$ cm. The maximum growth rates for three cases appear approximately in the neighborhood of $y = 0.5$, and the growth rates shows asymmetrical patterns, which indicate the occurrence of either one single or more than one convective cell. At $y = 0.5$, the maximum growth rate for $10g_0$ is nearly greater than for $1g_0$ by a factor of 2. Near at $y = 2.0$ the growth rates follow in the order of $10g_0 < 4g_0 < 1g_0$, which reflect intensive convective flow fields with increasing the gravity acceleration up to $10g_0$. As shown in Fig. 6, like the cases of $\Delta T = 30$ K the maximum growth rates for three gravity accelerations appear at in the neighborhood of $y = 0.5$, and the growth rates versus the interfacial positions show asymmetrical against at $y = 1.0$. The growth rates for three different gravities of 1, 4, $10g_0$ approach at the neighborhood of 0.3. Unlike the cases of $\Delta T = 30$ K, the near at $y = 2.0$ the growth rates for $\Delta T = 90$ K follow in the order of $1g_0 < 4g_0 < 10g_0$. In comparisons of Fig. 5

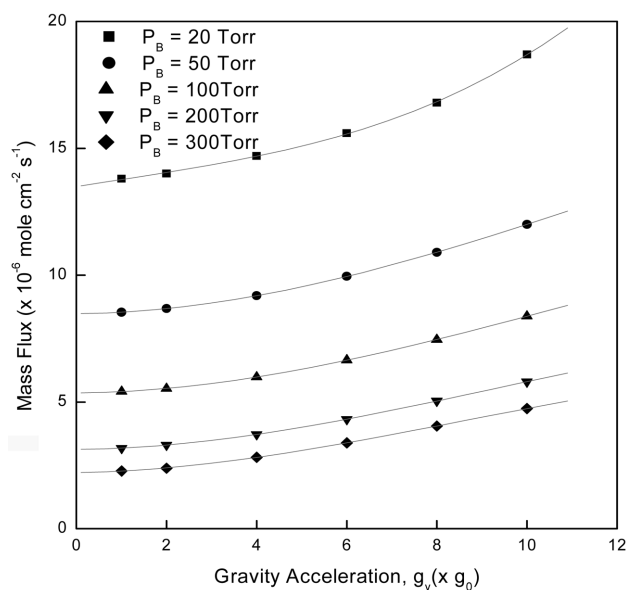


Fig. 7. Effects of partial pressure of component B, P_B (Torr) on the mass flux of Hg_2Cl_2 in terms of $\text{mole cm}^{-2} \text{s}^{-1}$ for various gravity accelerations of $1g_0 \leq g_y \leq 10g_0$ for the horizontal orientations and the temperature differences between the source and the crystal region of $320^\circ\text{C} \rightarrow 290^\circ\text{C}$, $Ar = 5$, $L = 10$ cm, with the linear temperature profiles at walls.

with Fig. 6, this discrepancy between $\Delta T = 30$ K and 90 K is likely to be due to the fact that near at $y = 2.0$ the patterns of growth rates for $\Delta T = 90$ K are more convection-dominated than for $\Delta T = 30$ K. As shown in Fig. 5, for $\Delta T = 30$ K and $10g_0$, the maximum growth rate is greater than the minimum growth rate by a factor of 2.7. On the other hand, as shown in Fig. 6, for $\Delta T = 90$ K and $10g_0$, the maximum growth rate is greater than the minimum growth rate by a factor of 4.9. Therefore, the deviation between the maximum and the minimum growth rate for $\Delta T = 90$ K and $10g_0$ is greater than for $\Delta T = 30$ K by a factor of 2, which indicate the mass transport is convection-dominated with increasing the temperature difference.

Fig. 7 shows effects of partial pressure of component B, P_B (Torr) on the mass flux of Hg_2Cl_2 in terms of $\text{mole cm}^{-2} \text{s}^{-1}$ for various gravity accelerations of $1g_0 \leq g_y \leq 10g_0$ for the horizontal orientations and the temperature differences between the source and the crystal region of $320^\circ\text{C} \rightarrow 290^\circ\text{C}$, $Ar = 5$, $L = 10$ cm, with the linear temperature profiles at walls. As shown in Fig. 7, the mass flux increases with increasing the gravity acceleration, for $1g_0 \leq g_y \leq 10g_0$, and decreases with increasing the partial pressure of component B, xenon (Xe), P_B . It is clear to see that as the P_B increases, the gap between the polynomial regression lines is decreased. Fig. 8 shows the $|U|_{\text{max}}$ as a function of gravity accelera-

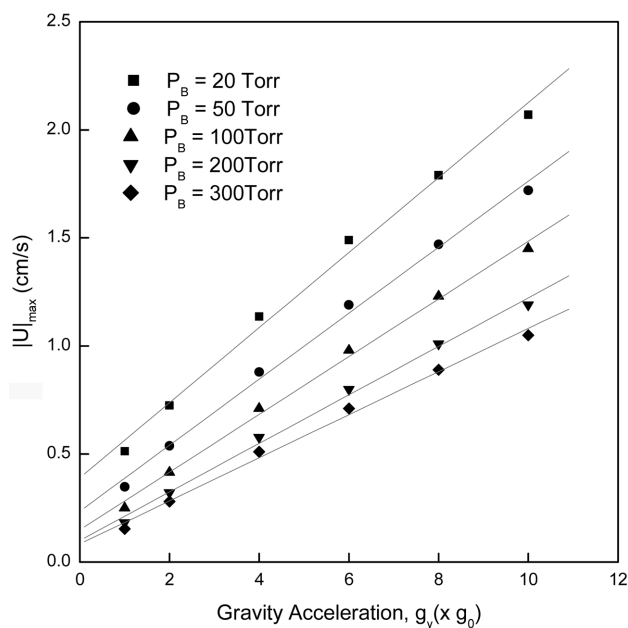


Fig. 8. The $|U|_{\max}$ as a function of gravity accelerations for various partial pressures of P_B (Torr), $20 \text{ Torr} \leq P_B \leq 300 \text{ Torr}$, corresponding to Fig. 7.

tions for various partial pressures of P_B (Torr), 20 Torr P_B 300 Torr, corresponding to Fig. 7. The $|U|_{\max}$ is directly proportional to the gravity acceleration for 20 Torr P_B 300 Torr. As the partial pressure of P_B (Torr) decreases from 300 Torr to 20 Torr, the slope of the $|U|_{\max}$ versus the gravity acceleration increases from 0.1 sec to 0.17 sec. For the gravity accelerations under consideration, the gap between the polynomial regression lines of the $|U|_{\max}$ is the smallest at $g_y = 1g_0$. In other words, at $g_y = 10g_0$, as the P_B (Torr) is increased from 20 Torr to 300 Torr, i.e. by a factor of 15, the $|U|_{\max}$ is decreased from 2.0 cm s^{-1} to 1.0 cm s^{-1} by a factor of 0.5. On the other hand, at $g_y = 1g_0$, as the P_B (Torr) is increased from 20 Torr to 300 Torr, i.e. by a factor of 15, the $|U|_{\max}$ is decreased from 0.5 cm s^{-1} to 1.5 cm s^{-1} by a factor of 0.33. Therefore, as the gravity level is decreased from $1g_0$ to $10g_0$, the ratio of factors for $|U|_{\max}$ is approximately 1.5, i.e. a factor of 0.5 to a factor of 0.33. Fig. 9 shows the crystal growth rate of Hg_2Cl_2 as a function of gravity accelerations for various partial pressures of P_B (Torr), $20 \text{ Torr} \leq P_B \leq 300 \text{ Torr}$, corresponding to Fig. 7. The growth rate increases the third order polynomially with the gravity level for $20 \text{ Torr} \leq P_B \leq 300 \text{ Torr}$. At $g_y = 10g_0$, as the P_B (Torr) is increased from 20 Torr to 300 Torr, i.e. by a factor of 15, the growth rate is decreased from 0.2 cm hr^{-1} to 0.05 cm hr^{-1} by a factor of 0.25. On the other hand, at $g_y = 1g_0$, as the P_B (Torr) is increased from 20 Torr to 300 Torr, i.e. by a factor of

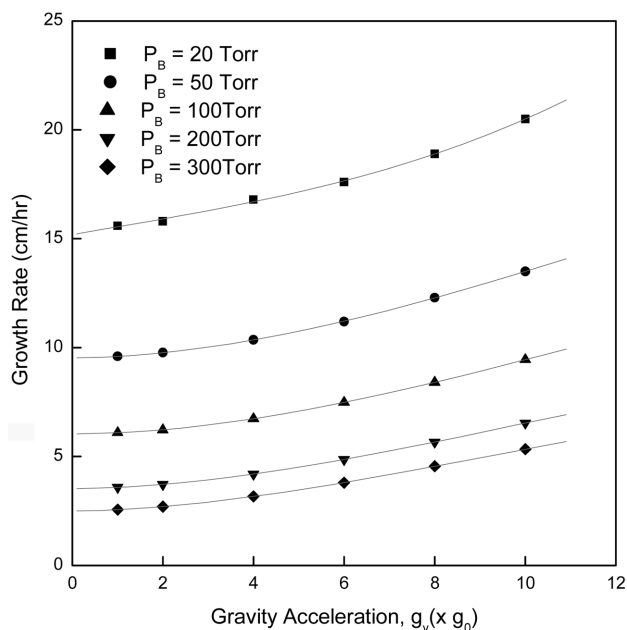


Fig. 9. The crystal growth rate of Hg_2Cl_2 as a function of gravity accelerations for various partial pressures of P_B (Torr), $20 \text{ Torr} \leq P_B \leq 300 \text{ Torr}$, corresponding to Fig. 7.

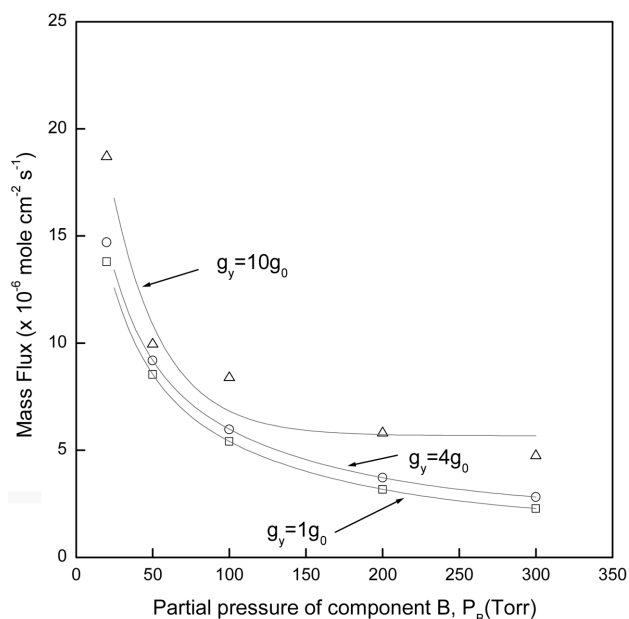


Fig. 10. The mass flux of Hg_2Cl_2 in terms of $\text{mole cm}^{-2}\text{s}^{-1}$ as a function of partial pressure of component B, P_B (Torr) for three gravity accelerations of $g_y = 1g_0, 4g_0$ and $10g_0$, corresponding to Fig. 7.

15, the growth rate is decreased from 0.15 cm hr^{-1} to 2.5 cm hr^{-1} by a factor of 0.06. Therefore, as the gravity level is decreased from $1g_0$ to $10g_0$, the ratio of factors for the growth rate is approximately 4, i.e. a factor of 0.25 to a factor of 0.06. Fig. 10 shows the mass flux of Hg_2Cl_2 in terms of $\text{mole cm}^{-2}\text{s}^{-1}$ as a function of par-

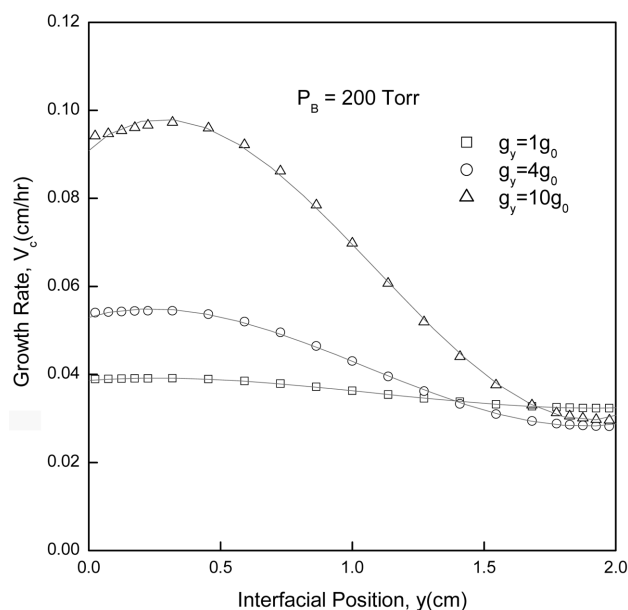


Fig. 11. Interfacial distributions of crystal growth rate of Hg_2Cl_2 for various gravity accelerations, at $\Delta T = 30$ K and $P_B = 200$ Torr. Based on $Ar = 5.0$, $Pr = 0.74$, $Le = 0.59$, $Gr_t = 1.4 \times 10^3$, $Gr_s = 1.1 \times 10^3$, $Pe = 0.8$, $C_v = 1.8$, $g_y = 1g_0$.

rial pressure of component B, P_B (Torr) for three gravity accelerations of $g_y = 1g_0$, $4g_0$, $10g_0$, corresponding to Fig. 7. The mass flux of Hg_2Cl_2 decreases exponentially with increasing the partial pressure of component B, P_B (Torr) from 20 Torr up to 300 Torr. Near at $P_B = 20$ Torr, the mass flux decreases sharply and, then since $P_B = 100$ Torr, decreases slowly until at $P_B = 300$ Torr. At $g_y = 10g_0$, the decrease in the mass flux appears relatively small for $100 \text{ Torr} \leq P_B \leq 300$ Torr. Figs. 5 and 12 show the interfacial distributions of crystal growth rate of Hg_2Cl_2 for various gravity accelerations, at $P_B = 20$ Torr and 200 Torr, respectively. For the case of $g_y = 1g_0$, $P_B = 20$ Torr and $\Delta T = 30$ K in Fig. 5, the corresponding parameters are as follows: $Ar = 5.0$, $Pr = 0.81$, $Le = 0.34$, $Gr_t = 8.4 \times 10^3$, $Gr_s = 9.7 \times 10^4$, $Pe = 2.38$, $C_v = 1.1$. As shown in Fig. 11, like the cases of $P_B = 20$ Torr, in Fig. 5, the maximum growth rates for three gravity accelerations appear at the neighborhood of $y = 0.5$, and the growth rates versus the interfacial positions show asymmetrical against at $y = 1.0$. The growth rates for three different gravities of 1, 4 and $10 g_0$ approach at the neighborhood of 0.043. Unlike the cases of $P_B = 20$ Torr, the near at $y = 2.0$ the growth rates for $P_B = 200$ Torr follow in the order of $4g_0 < 10g_0 < 1g_0$. In comparisons of Fig. 5 with Fig. 11, this discrepancy between $P_B = 20$ Torr and 200 Torr is likely to be due to the fact that near at $y = 2.0$ the patterns of growth rates for $P_B = 20$ Torr are more convection-dominated than for $P_B =$

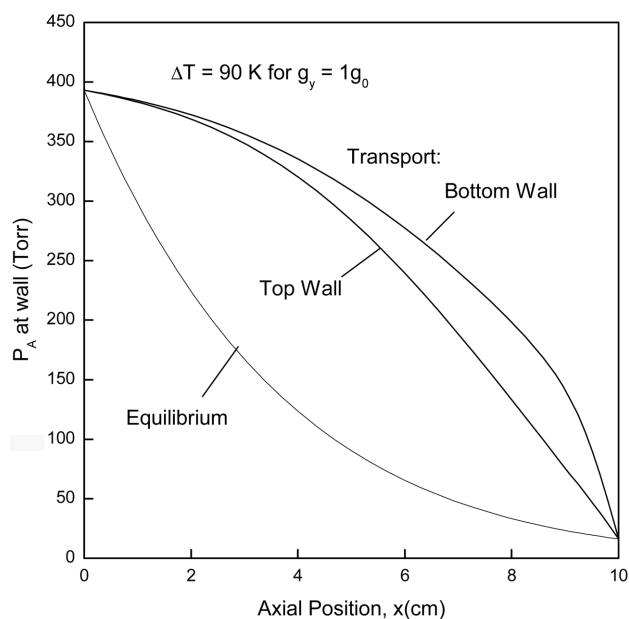


Fig. 12. Axial distribution of partial pressures of component A (Hg_2Cl_2) at the walls resulting from diffusive-convective transport at $g_y = 1g_0$, $\Delta T = 90$ K ($350^\circ\text{C} \rightarrow 260^\circ\text{C}$) and equilibrium vapor pressure profile corresponding to the linear wall temperature distribution. Based on $Ar = 5$, $P_B = 20$ Torr, $Ar = 5$, $L = 10$ cm.

200 Torr. The maximum growth rate for $P_B = 20$ Torr and $10g_0$ in Fig. 5 is greater than the minimum growth rate by a factor of 2.7. On the other hand, the maximum growth rate for $P_B = 200$ Torr and $10g_0$ in Fig. 5 is greater than the minimum growth rate by a factor of 3.34. Therefore, the deviation between the maximum and the minimum growth rate for $P_B = 200$ Torr and $10g_0$ is greater than for $P_B = 20$ Torr by a factor of 1.23, which implies the mass transport is convection-dominated with increasing the partial pressure of component B, P_B .

Fig. 12 shows the axial distribution of partial pressures of component A (Hg_2Cl_2) at the walls resulting from diffusive-convective transport at $g_y = 1g_0$, $\Delta T = 90$ K ($350^\circ\text{C} \rightarrow 260^\circ\text{C}$) and equilibrium vapor pressure profile corresponding to the linear wall temperature distribution. In Fig. 12, we compare the equilibrium profile with the $p_A(y)$ s that arise at the bottom and the top walls due to diffusive-convective transport at $1g_0$. It should be noted that the higher concentration along the bottom wall, again reflecting the counter-clockwise sense of rotation of the thermal and/or solutal convection. The vapor of component A (Hg_2Cl_2) is in the supersaturated state throughout the ampoule in both cases, so it is easy to see why a linear temperature profile is rarely used in practice.

4. Conclusions

The roles of convection in crystal growth of Hg_2Cl_2 -Xe can be enlarged in physical vapor transport systems for normal and high gravity environments. A gravitational acceleration level of more than $1g_0$ can be adequate to ensure diffusive-convection transport. The operating conditions under consideration in this study are $\text{Ar} = 5$, $P_B = 20$ Torr, $\text{Ar} = 5$, $L = 10$ cm, $\Delta T = 90$ K and $g_y = 1g_0$, with the linear temperatures on the walls. The governing dimensionless parameters are as follows: $\text{Ar} = 5.0$, $\text{Pr} = 0.78$, $\text{Le} = 0.5$, $\text{Gr}_l = 5.6 \times 10^4$, $\text{Gr}_s = 4.0 \times 10^5$, $\text{Pe} = 4.13$, $C_v = 1.1$. For both $\Delta T = 60$ K and 90 K, the mass flux increases by a factor of 3 with increasing the gravity acceleration from $1g_0$ up to $10g_0$. On the other hand, for $\Delta T = 30$ K, the flux is increased by a factor of 1.36 for the range of $1g_0 \leq g \leq 10g_0$. Consequently, under the conditions of high gravity accelerations, the mass fluxes for both $\Delta T = 60$ K and 90 K are approximately greater than the flux at $\Delta T = 30$ K by a factor of 2. The maximum growth rates for $1g_0$, $4g_0$ and $10g_0$ appear approximately in the neighborhood of $y = 0.5$, and the growth rates shows asymmetrical patterns, which indicate the occurrence of either one single or more than one convective cell. The maximum growth rate for $10g_0$ is nearly greater than that for $1g_0$ by a factor of 2.0 at $P_B = 20$ Torr. For three different gravity levels of $1g_0$, $4g_0$ and $10g_0$, the maximum growth rates are greater than the minimum rates by a factor of nearly 3.0 for $P_B = 20$ Torr. The mass flux increases with increasing the gravity acceleration, for $1g_0 \leq g_y \leq 10g_0$, and decreases with increasing the partial pressure of component B, xenon (Xe), PB. The $|U|_{\max}$ is directly proportional to the gravity acceleration for $20 \text{ Torr} \leq P_B \leq 300$ Torr. As the partial pressure of P_B (Torr) decreases from 300 Torr to 20 Torr, the slope of the $|U|_{\max}$ versus the gravity acceleration increases from 0.1 sec to 0.17 sec. The mass flux of Hg_2Cl_2 is exponentially decayed with increasing the partial pressure of component B, P_B (Torr) from 20 Torr up to 300 Torr.

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