Estimation of the Diffusion Coefficient of GaSb into InGaSb Melt using Bayesian Optimization Method and the ISS Experimental Results

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Introduction

$In_xGa_{1-x}Sb$

Promising semiconductor controllable composition → Adjustable Lattice parameter & wave length → Photonic & electronic devices, energy conversion applications (TE, TPV)

Under 1G : Convection & Diffusion simultaneously

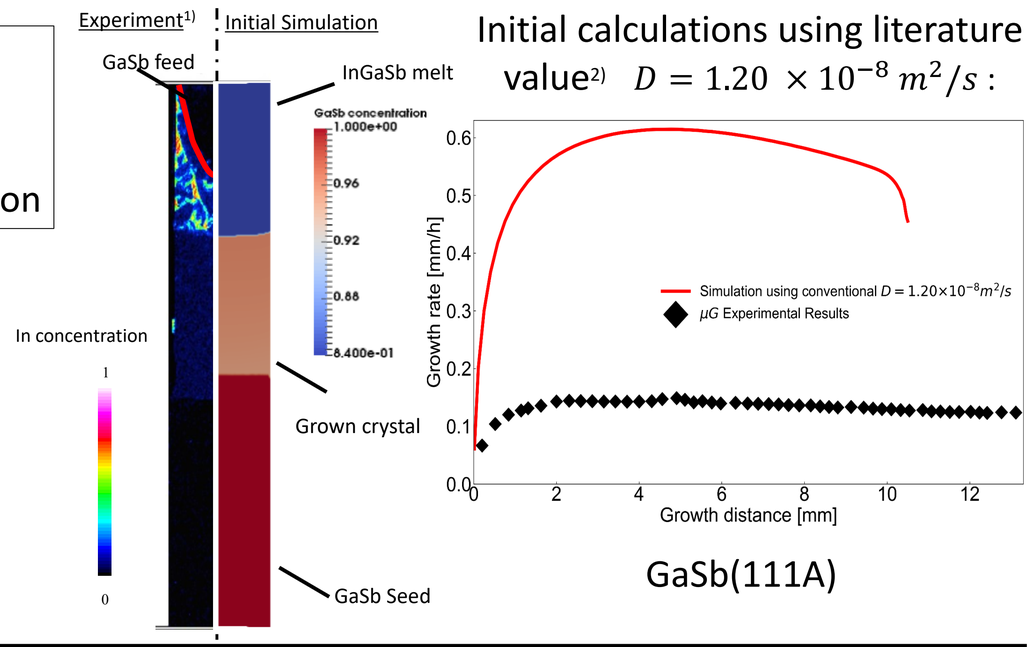
Under μ-G: Diffusion phenomena only → **Less complex to analyze under μ-G**

The simulation results do not match the experimental ones :
- Much larger growth rate
- Excessive GaSb feed dissolution

Since diffusion phenomena only

⬇

D value might be too large



Initial calculations using literature value[2)] $D = 1.20 \times 10^{-8}\ m^2/s$:

GaSb(111A)

Objective

Estimate D using the ISS experimental results, numerical simulations and Bayesian optimization method.

1) Y. Inatomi, K. Sakata, M. Arivanandhan, G. Rajesh, V.N Kumar, T. Koyama, Y. Momose, T. Ozawa, Y. Okano, and Y. Hayakawa: npj Microgravity, **1** (2015) 15011.

2) C. Stelian, T. Duffar and I. Nicoara: J. Cryst. Growth **255** (2003) 40.

Numerical Method

Governing Equations

In the Crystal Region

$$\nabla . \boldsymbol{v} = 0$$

$$\frac{\partial \boldsymbol{v}}{\partial t} + (\boldsymbol{v} . \nabla)\boldsymbol{v} = -\frac{1}{\rho}\nabla p + \nu\nabla^2 \boldsymbol{v} + \boldsymbol{g}(\beta_T \Delta T + \beta_C \Delta C)$$

$$\frac{\partial T}{\partial t} + (\boldsymbol{v} . \nabla)T = \alpha\nabla^2 T$$

$$\frac{\partial C}{\partial t} + (\boldsymbol{v} . \nabla)\mathrm{C} = D\nabla^2 C$$

In the Outer Region

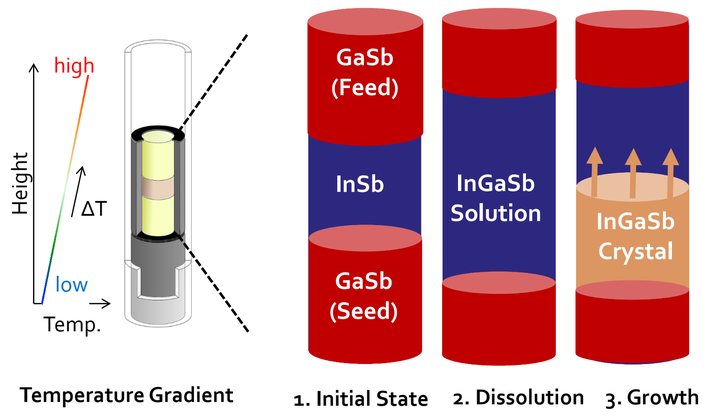
$$\frac{\partial T}{\partial t} = \alpha_i \nabla^2 T \qquad i \text{ Subscript standing for BN and Quartz}$$

Nomenclature

$\boldsymbol{v}$: Velocity [m/s]
t : Time [s^{-1}]
ρ : Density [kg/m^3]
p : Pressure [$kg/m \cdot s^2$]
ν : Kinematic viscosity [m^2/s]
$\boldsymbol{g}$: Gravitational acceleration [m/s^2]
β_T : Thermal expansion coefficient [K]
β_C : Solutal expansion coefficient [-]
T : Temperature [K]
α : Thermal diffusivity [m^2/s]
C : Average concentration of the solid-liquid mixture [-]
D : Diffusion coefficient [m^2/s]

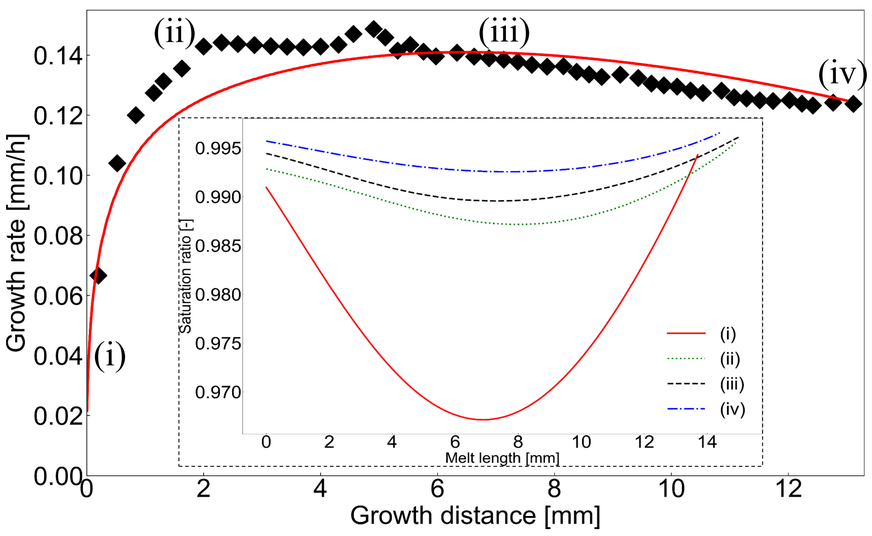
Experimental Setting

Vertical Temperature Gradient Method



Results & Discussion

Results for $D = 2.20 \times 10^{-9}\ m^2/s$



Due to the change in melt saturation ratio, We consider the effect of GaSb concentration on D by introducing the following equation :

$$D = D_0 \cdot e^{(b \cdot C)}$$

Using Bayesian Optimization algorithm, We look for the best combination of D_0 and b

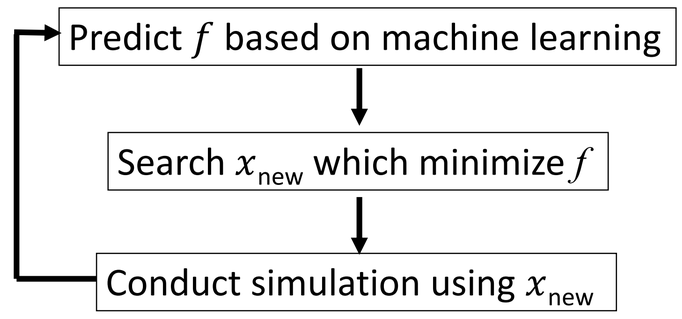
Bayesian Optimization

-Search the parameter x which minimizes the objective function f by using predicted mean value and standard deviation.

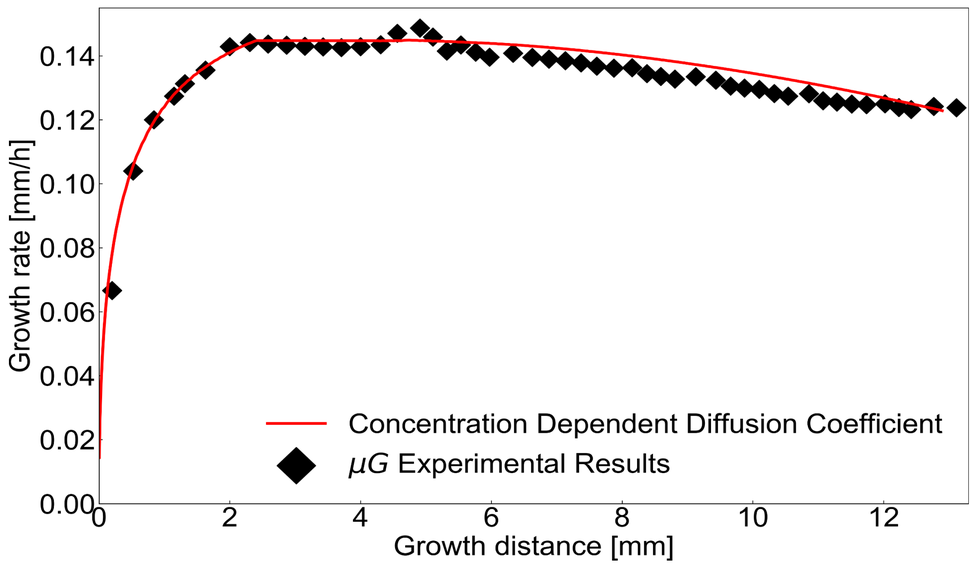
$$f(x) = \frac{1}{L}\int \left(V_{\mathrm{sim}} - V_{\mathrm{exp}}\right)^2 dL \qquad x = \begin{pmatrix} D_0 \\ b \end{pmatrix}$$

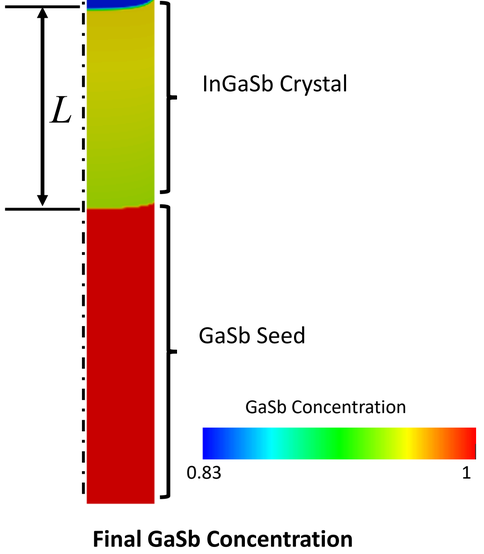
V_{exp}: Growth rate from the experiment
V_{sim}: Growth rate from the simulation
L: Growth distance

Algorithm

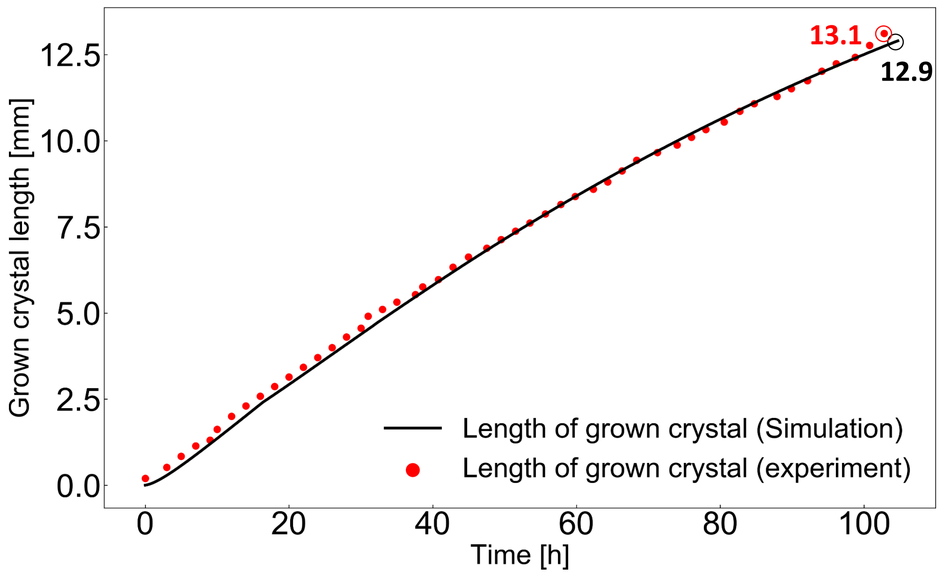


After optimization → $D = 2.70 \cdot 10^{-8} \cdot e^{-3C}$





Final GaSb Concentration



Conclusion

A relationship between the concentration and the diffusion coefficient of GaSb into InGaSb melt was established based on the ISS experimental results and Bayesian optimization methods. It is concluded that the growth rate, feed/seed dissolutions lengths and grown crystal length are strongly affected by the diffusion coefficient and therefore GaSb concentration in the melt.

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