Journal of Korean Association of Crystal Growth
Vol. 9, No. 4 (1999) 381-383

Macroscopic and microscopic mass transfer in silicon czochralski method

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(Received June 9, 1999)

Abstract First topic of this paper aims to clarify how oxygen and heat transfer in silicon melt under cusp-shaped magnetic fields. We obtained asymmetric temperature distribution by using time dependent and three-dimensional calculation. Second topic is study on molecular dynamics simulation, which was carried out to estimate diffusion constants of oxygen in silicon melt.

1. Introduction

Oxygen in silicon single crystals plays an important role for purifying impurity in the grown crystals. Since lack of the concentration enhances formation of slip in the wafers, precise control of oxygen concentration in the crystals should be requested to obtain appropriate concentration for getting impurity in the wafer. Oxygen atoms incorporate into the crystals by convective and diffusive transfers in the melt. Many papers reported upon convection in the melt so far, although only few paper on oxygen-transfer mechanism under cusp-shaped magnetic fields [1]. Concerning diffusion coefficient of oxygen in the melt, few papers have been discussed so far.

This paper aims to clarify how oxygen is transferred in silicon melt under cusp-shaped magnetic fields, and to obtain diffusion constant of oxygen in the melt using molecular dynamics simulation.

2. Oxygen transfer under cusp-shaped magnetic fields

Three-dimensional and time dependent calculation was carried out to obtain three-dimensional distribution of oxygen in silicon melt under cusp-shaped magnetic fields. Diameters of crucible and crystal were set to 7.5 cm and 3.75 cm, respectively. Magnetic-field distribution used in this study is shown in Fig. 1. Calculated result shows asymmetric velocity and tem- perature distributions in the various height of the melt shown in Fig. 2. The asymmetric temperature distribution was due to flow instability with asymmetric flow pattern [2].

Figure 3 shows oxygen distribution in silicon melt at various height of the melt. We can find an asymmetric distribution, which is more complicated structure due to low diffusivity of oxygen in the melt. The result indicates that magnetic fields are not always stabilize melt convection, therefore, appropriate distribution of magnetic fields should be selected.

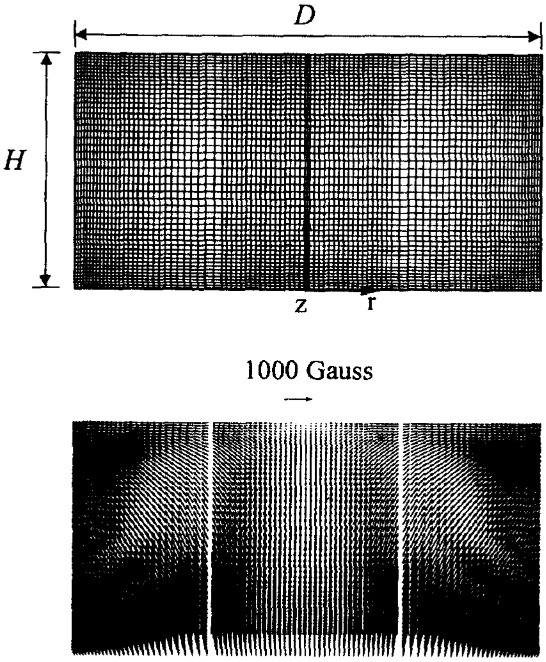

Fig. 1. Grid and cusp-shaped magnetic field imposed with its symmetry plane equal to the free surface of the melt in the r-z plane.

3. Molecular dynamics simulation

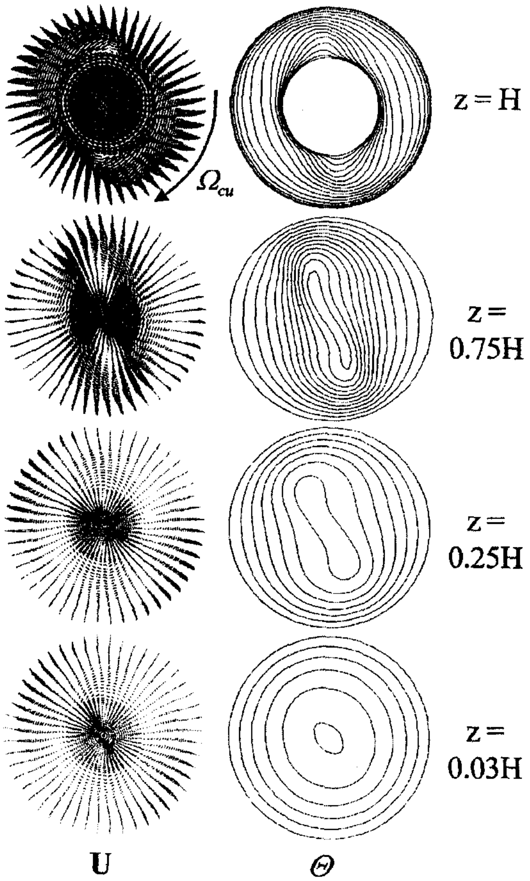

Fig. 2. Velocity observed from rotating frame and temperature distribution at various height.

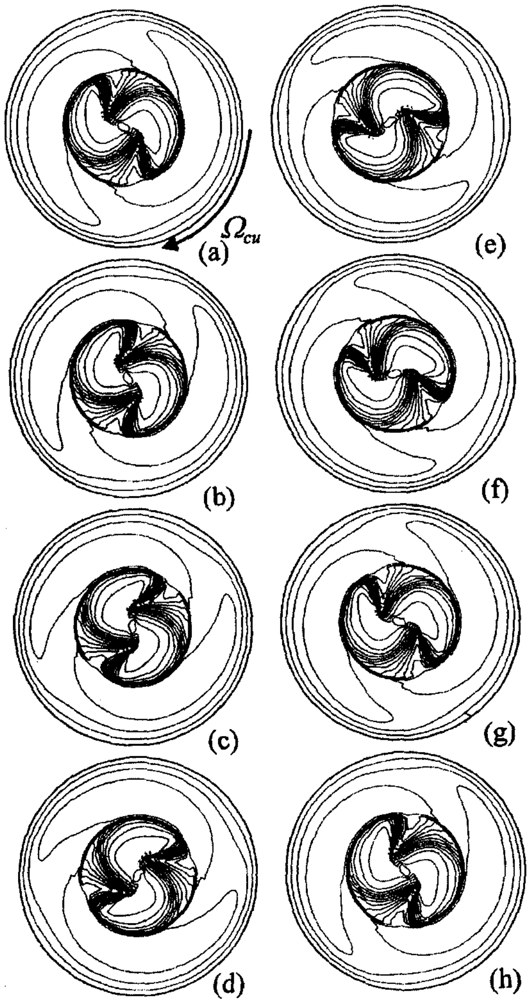

Fig. 3. Oxygen concentration distribution at various height.

The potential used in the present calculation contains modified Stillinger-Weber potential, van Beest potential and ionization energy potential developed by Jiang and Brown [3]. This includes Si-Si, Si-O, and O-O interactions in the forms of two and three body potential with a competition between the ionic and covalent character of chemical bonding. Detail of this calculation is reported elsewhere [4].

Figure 4 shows projection of an oxygen atom and 216 silicon atoms observed from <001> direction at a temperature of 1000 K. The atom enclosed by a circle in the figure corresponds to an oxygen atom, therefore, we can recognize that the oxygen atom settled in an interstitial site.

Main object of the present study is to estimate a diffusion constant of oxygen atom in silicon melt. Temperature of the system with one oxygen and 216 silicon atoms was elevated until 1700 K, then, displacements of oxygen atom and silicon atoms were obtained to estimated diffusion constant of oxygen and silicon atoms using eq. (1),

$$D=\frac{1}{6}\lim_{\Delta t\to\infty}\frac{\langle (x-x_0)^2\rangle}{\Delta t} \tag{1}$$

where x, x_0 and Δt are position of atoms at a specific time, initial position and time difference, respectively.

Figure 5 shows square displacements of oxygen atom and silicon atoms as a function of time. Oxygen diffusion constant was obtained in an elevated temperature of 1700 K using results shown in Fig. 5. Calculated diffusion constant of oxygen in the melt was about 2×10^{-4} cm^2/sec, which is almost the same order of diffusion constant of pure silicon. The result can be

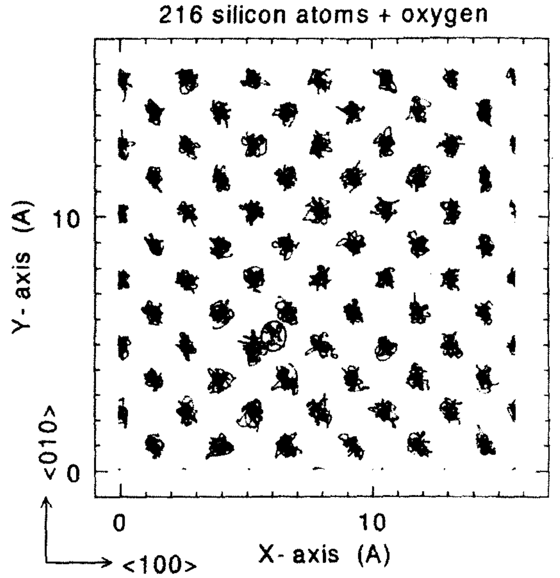

Fig. 4. Projection image of an oxygen atom and 216 silicon atoms observed from <001> direction at a temperature of 1000 K.

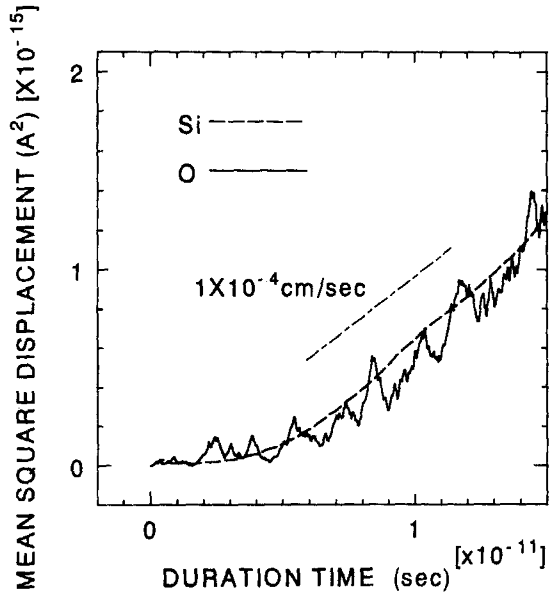

Fig. 5. Square displacement of oxygen and silicon atoms as a function of time.

obtained from the result with the same gradients of the lines of oxygen and silicon shown in Fig. 5, although data of oxygen is scattered due to smaller number of atom than that of silicon.

4. Summary

Time-dependent three-dimensional calculation was carried out to clarify how oxygen transfers in the melt under cusp-shaped magnetic fields. We obtained asymmetric oxygen concentration in the melt by using the calculation.

Molecular dynamics simulation was carried out to estimate a diffusion constant of oxygen in silicon melt. To confirm a validity of the present molecular dynamics code, vibration frequencies of oxygen in pure silicon and V-O pair were calculated. Calculated frequencies of oxygen in pure silicon and V-O pair are 1000 cm^{-1} and 800 cm^{-1}, respectively. Calculated diffusion constant of oxygen in silicon melt is about 2×10^{-4} cm^2/sec.

Acknowledgement

This work was conducted as JSPS Research for the Future Program in the Area of Atomic-Scale Surface and Interface Dynamics.

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