

Visualization of Large-scale Atomic Interactions during the Melting and Crystallization Process

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Introduction

The visualization and simulation of atomic-scale material model capable of melting, crystallization and amorphization has been developed. The large-scale molecular-dynamics (MD) calculations are done to examine crystal growth and defect formation process from the melted silicon (Si) based on the ordinary Langevin equations of motion. The developed computer system enables us interactive visualization of solid/liquid interface structures responding to the control parameters such as the temperature gradient and pulling speed. The particle objects representing up to 10^4 atoms in an interactive 3D environment model material behaviour. A particle in proposed dynamic system interacts through attractive covalent forces and short-range repulsion forces. This research was conducted to understand the processes that can control the quality of single-crystal silicon (Si) grown from the melt by Czochralski crystal puller, shown in Figure 1.

Simulation method

The motion of the particle i is governed by the Langevin equation of motion

$$\dot{\mathbf{x}}_i(t) = \mathbf{v}_i(t), \quad m_i \dot{\mathbf{v}}_i(t) = -m_i \gamma_i \mathbf{v}_i(t) + F_i(\{\mathbf{x}(t)\}) + R_i(t) \quad (1)$$

where \mathbf{x}_i , \mathbf{v}_i , m_i , and $\lambda_i = 5ps^{-1}$, are the position, velocity, atomic mass and friction coefficient of the i -th particle at time t , respectively. The inter-atomic force F_i between N particles is derived from the Tersoff [1] potential of Si, the stochastic force R_i was introduced to mimic the motion of solvent molecules on the solute, it also serves as temperature controller in the system. The stochastic numerical integration of the third order [2] was performed under the constant volume within the cubic domain with periodic boundary conditions on side faces and a reflection plane on bottom. At each time step (0.002 ps) the collision between the particle and the reflection plane is calculated to prevent particle from escaping out of the volume.

Results

Figure 2 shows the simulated crystal growth process with a pulling speed of 5 m/s in the [111] direction. Joining two heated crystalline Si cells made initial states. The former cell had density of crystal Si, 2.33 g/cm^3 and the later did 2.57 g/cm^3 , which gives the density of liquid Si structure. Calculated growth rate and pulling speed are much larger then in a real crystal puller because much larger volume and longer time period is needed to get exact results. Nevertheless, the proposed simulation system of crystallization process is useful to analyse crystal growth rates. To further study the effects of impurities on a crystal growth and defects formation we show the simulation of Si cluster interaction with oxygen atoms on Figure 3.

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References

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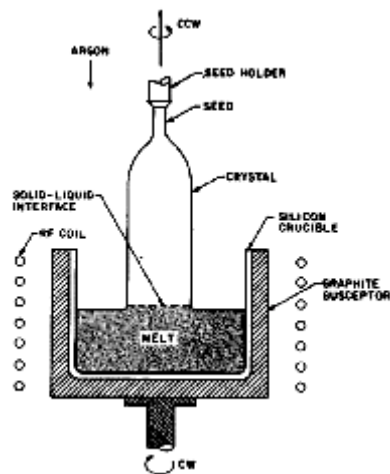


Figure 1. Czochalski crystal puller.

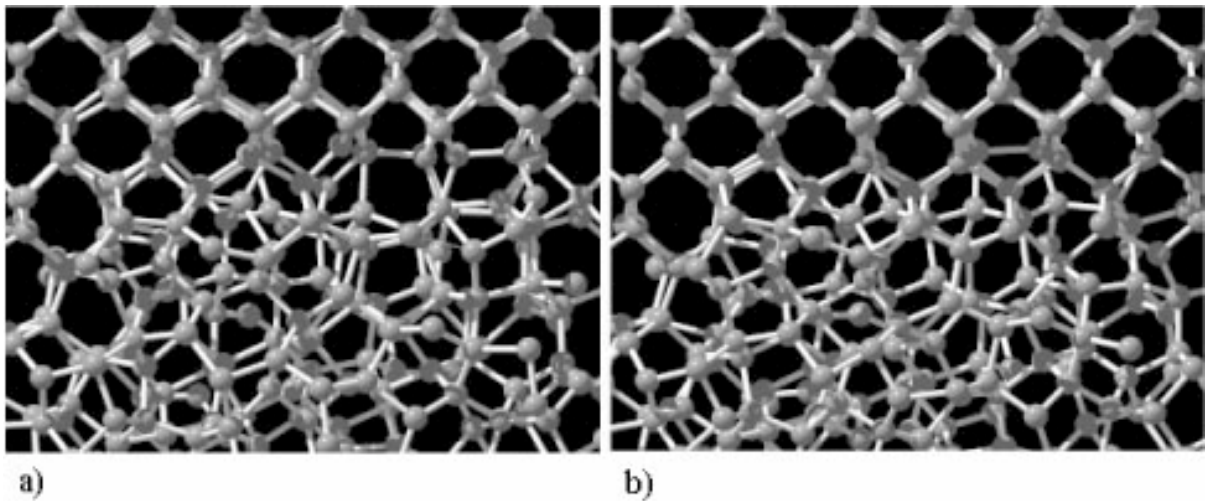


Figure 2. An example of atomic arrangements within the crystal/liquid interface during the crystallization process after simulation time of a) 300 ps and b) 600 ps.

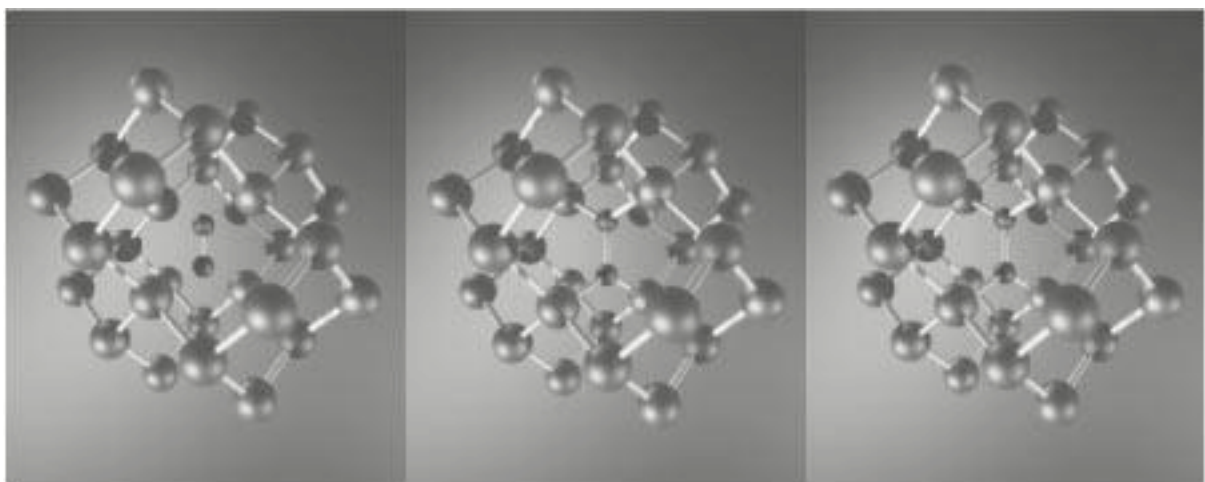


Figure 3. Oxygen and silicon interactions (Si_{28}O_2). Two oxygen atoms are located at the centre.