

# Molecule Dynamics Calculation on Formation of Void Defects in Si and Ge Crystals

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## 1 Introduction

In recent years, Large Scale Integration (LSI) devices have been developed with downsizing. In this technology trend, high quality and large diameter Si wafers are used as substrates with controlling the point defects. It is well known that void defects are formed by the vacancy aggregation in Si during crystal growth. Since the void defects at the Si wafer surface degrade the LSI performance, it is important to understand the formation mechanism of vacancies.

Furthermore, Ge crystal is under consideration for the LSI substrate as the carrier mobility in Ge is higher than that in Si<sup>[1]</sup>. In recent studies, void defects with larger sizes are found in Ge crystals compared to Si crystals<sup>[2]</sup>. However, the mechanism of the void formation in Ge crystals is not fully understood. In this study, the formation of void defects in Si and Ge crystals was analyzed by molecule-dynamics (MD) simulations.

## 2 Calculation detail

Figure 1 shows the calculation cell of 1000 atoms for Si and Ge crystals. The side length of the cell is 27.154 Å (Si) and 28.285 Å (Ge). One vacancy is introduced at the center of the cell by removing one atom. Furthermore, the nearest atoms were eliminated one by one, and voids with different sizes up to including 17 vacancies are modeled. The three dimensional periodic boundary condition was imposed. Materials Explorer of Fujitsu Ltd. for Molecular-dynamics simulation was used in this study<sup>[3]</sup>. The Tersoff potential was used with an ensemble of NTV. Formation energy of void was calculated from the obtained internal energy of the cell.

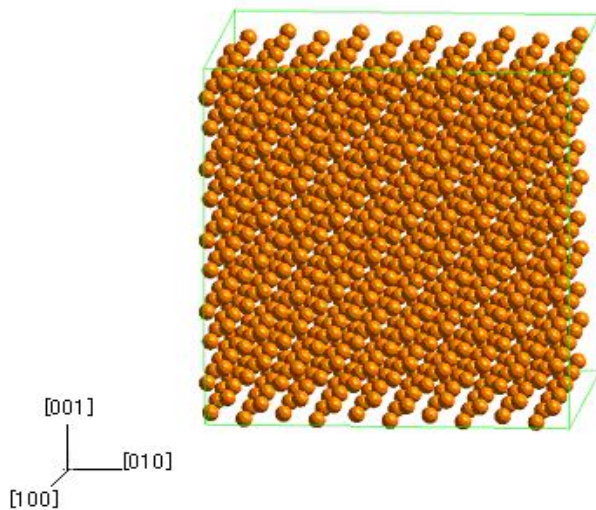


Fig.1 MD calculation cell including 1000 atoms.

Formation energy  $E_f(N)$  of void including the  $N$  vacancies( $V$ ) was obtained with equation (1).

$$E_f(N) = E_N - (1000 - N)E_0 / 1000 \quad (1)$$

Here,  $E_0$  is the internal energy of the perfect cell.

## 3. Calculation results and discussion

### 3.1 Calculation results of formation energy $E_f(N)$

Figure 2 shows the calculated  $E_f(N)$  of void in Si and Ge crystals.

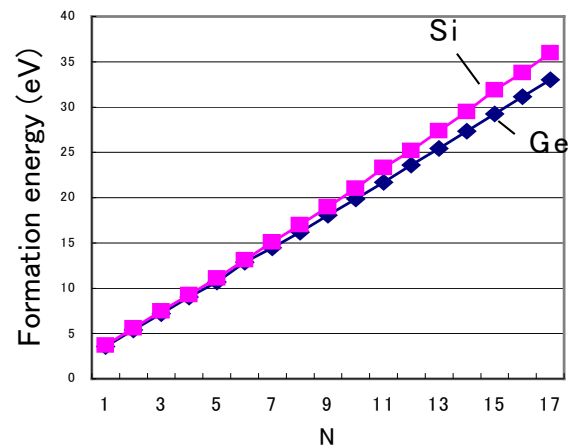


Fig.2 Calculated  $E_f(N)$  of Si and Ge crystals.

It was found that the formation energy of one vacancy is 3.70 eV (Si) and 3.58 eV (Ge), respectively. Furthermore, the energy of the void formation in Ge crystal is found to be lower than that in Si crystal.

Next, the binding energy of void and one vacancy was obtained with equation (2).

$$E_b(N+1) = (E_N + E_1) - (E_{N+1} + E_0) \quad (2)$$

The calculated results from  $E_b(2)$  to  $E_b(17)$  are shown in Fig. 3.

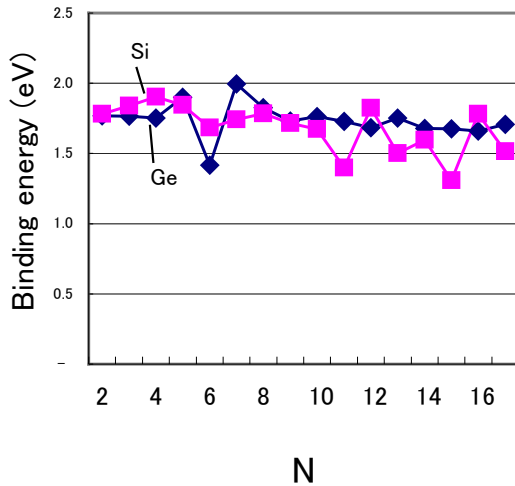


Fig.3 Calculated  $E_b(N)$  of Si and Ge crystals.

It was found that the average binding energy of void and one vacancy from N=1 to N=17 is 1.74 eV (Si) and 1.68 eV (Ge), respectively.

### 3.2 Interaction of void and vacancy

Here, we calculated the internal energy of the cell with one V approaching to the void including 4 vacancies. In this study,  $E_i(1)$  is the internal energy of one V at the nearest to the void, and  $E_i(2)$  is the internal energy of one vacancy which is at the second nearest to the void. In this way, the calculation was performed with L=1 to L=9, and the results are shown Fig. 4.

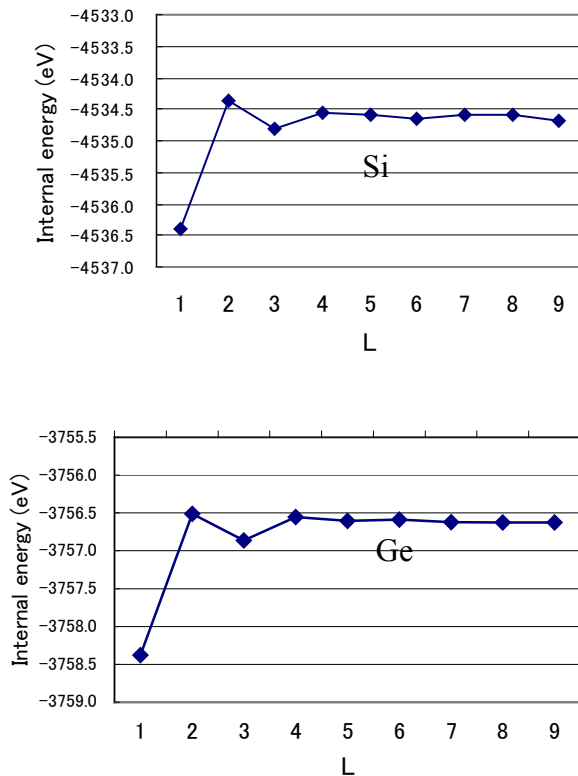


Fig.4 interaction four V and void

It was found that the vacancy should not be isolated but to be incorporated into void.

### 4. Conclusion

In this study, we have analyzed the formation of void defect in Si and Ge crystals by molecule-dynamics calculation. The obtained results are summarized as follows.

(1) Formation energy of one vacancy is 3.70 eV (Si) and 3.58 eV (Ge), respectively. Furthermore, the energy of the void formation in Ge crystal is found to be lower than that in Si crystal.

(2) The average binding energy of void and one vacancy from N=1 to N=17 is 1.74 eV (Si) and 1.68 eV (Ge), respectively.

(3) The vacancy should not be isolated but to be incorporated into void.

### Reference

- [1] C. Claeys and E. Simoen, Germanium-based Technologies: From Materials to Devices, Elsevier, Amsterdam, 2007
- [2] J. Vanhellefont, P. Spiewak, K. Sueoka and I. Romandic, *Phys. Status Solidi C* **6**, 1906–1911, 2009
- [3] Materials Explorer  
["http://www.cache.fujitsu.com/materialsexplorer/index.shtml"](http://www.cache.fujitsu.com/materialsexplorer/index.shtml)