Thermal equilibrium point defects in Si

Suezaw M[1], Iijima Y[1], Yonenaga I[1]*
*lead presenter: yonenaga@im.tohoku.ac.jp
1 Tohoku University, Japan

We determined temperature dependencies of concentrations of thermal equilibrium vacancies and interstitials in Si from the analyses of self-diffusion coefficients and their diffusion coefficients together with experimental quenching. The concentration of thermal equilibrium vacancies and interstitials at temperature T(K) are $\exp(6.5)\exp(-3.85\text{eV}/k_BT)$ and $\exp(10.6)\exp(-4.3\text{eV}/k_BT)$, respectively. The diffusion coefficients of vacancies and interstitials are determined to be $2.7\times10^{-3}\exp(-0.45\text{eV}/k_BT)$ and $2.5\times10^{-2}\exp(-0.49\text{eV}/k_BT)$ cm^2/s, respectively.[1, 2]

The results give an experimental answer to the point defect formation and migration, a long-standing and inexhaustible topic in Si since 1950's and also basic knowledge for crystal growth experimentally and theoretically. The thermal equilibrium concentration of interstitials at the melting point is 2.9×10^{14} cm^{-3}, higher than vacancies (1.1×10^{14} cm^{-3}). This leads to a question against the Voronkov's model widely accepted for phenomenological explanation of secondary defect development of excess vacancy- or interstitial-related induced at the liquid/solid interface during Si crystal growth.[3] Also, the difference of the formation energy of a vacancy and an interstitial makes a reconsideration whether the nature of thermal equilibrium point defects in Si are Frenkel pairs or Schottky defects.[4] The determined formation entropy of vacancies confirms that they might be point-like, not extended point defect.[5] The migration energies of vacancies and interstitials evaluated to be around 0.5 eV give some questions on previous analyses of diffusion experiments. In addition, the entropy for a vacancy migration is found to be negative.

The present results determined experimentally can address theoretical studies, including first-principles calculations of point defect formation and migration in Si crystal, soon. In addition, these can provide novel knowledge for controlling or eliminating secondary defects formed during crystal growth.

References

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