Activation energies of self-diffusion mediated by vacancies and interstitials in a high-purity Si crystal

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Two diffusion mechanisms, namely, the vacancy- and the interstitial-mediated mechanism, have been proposed to be active in Si crystal. To identify the diffusion mechanism, the diffusion constant of self-diffusion has so far been studied, based on the measurements of temperature dependence of the self-diffusion constant. It should be, however, difficult to determine the diffusion mechanism in such approaches.

To clarify the microscopic diffusion mechanism, it is necessary to determine the formation and the migration energy of a relevant point defect (i.e., vacancy or interstitial). To determine the formation energy of a vacancy, for example, we need to know the dependence of vacancy concentration on the heat-treated temperature. Within our knowledge, there seems no experimental method to detect isolated vacancies with low concentration. We propose a new quenching method; namely, specimens are heat-treated in hydrogen gas atmosphere, followed by quenching in water [1]. Instead of isolated vacancies, we can detect complexes of vacancy and hydrogen atoms, which are formed during quenching, by optical absorption measurement of hydrogen vibrations in the complex.

Recently we succeeded in estimating two activation energies of vacancy-mediated (4.3 eV) and interstitial-mediated (5.3 eV) self-diffusion from the formation and migration energies of a vacancy and an interstitial in high purity Si. Those energies were determined from the detection of complexes of point defects and hydrogen atoms by optical absorption measurement.