ATOMIC DIFFUSION IN SILICON

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We present a unified description of atomic diffusion processes in silicon, based on the results of parameter-free total-energy calculations. A consistent interpretation of both low- and high-temperature data is provided without the need to invoke a change in the nature of intrinsic defects as a function of temperature. The self-interstitial has negative-U properties and can migrate athermally via the Bourgoin-Corbett mechanism along several paths. Both vacancies and self-interstitials mediate self-diffusion with activation energies within the range of observed values. Both intrinsic defects also mediate the diffusion of impurities such as Al and P, but the detailed mechanisms are considerably more complex than those of self-diffusion.

I. INTRODUCTION

Atomic diffusion is an important solid-state process that is poorly understood in semiconductors, especially Si.[1,2] We distinguish two general types of atomic diffusion: Diffusion of atoms that normally occupy substitutional sites (e.g., Si atoms in Si, i.e., self-diffusion, and substitutional impurities such as P, Al, etc.), and diffusion of atoms which either normally occupy interstitial sites or have been dislodged from normal lattice sites by electron irradiation or some other means. Self-diffusion and substitutional-impurity diffusion are generally believed to be mediated by thermally created intrinsic defects such as vacancies, self-interstitials, etc., but no consensus has been achieved so far about either the nature of these defects or the details of the diffusion mechanisms.

During the last few years, a number of groups have developed and implemented practical methods for parameter-free calculations of the key quantities that underlie the interpretation of diffusion data, namely equilibrium configurations of defects, lattice relaxation, formation and migration energies, barrier changes caused by carrier capture, etc.[3-10] Results of these calculations have led to new insights regarding atomic migration and diffusion processes in Si, detailed answers to long-standing questions, and the reconciliation of seemingly inconsistent data. In this paper, we will review briefly the relevant experimental data and the interpretations proposed prior to the advent of parameter-free calculations, describe the new advances achieved with the use of parameter-free calculations (published or received in preprint form prior to this conference), and report new results regarding the high-temperature diffusion of dopant impurities in Si. We, thus, arrive at a unified description of high-temperature self-diffusion and impurity diffusion, and the low-temperature migration of interstitial atoms.

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