II. BRIEF REVIEW OF EXPERIMENTAL DATA

At low temperatures (<70 K), experimental data are available for vacancies and self-interstitials created by electron irradiation.[11] Vacancies created in this way have been identified and their migration barriers have been found to be small, 0.2 to 0.3 eV, depending on the charge state. Self-interstitials, on the other hand, have not been detected directly, but experimental data on p-type Si at very low temperatures (~4 K) strongly suggest that self-interstitials migrate athermally.[11] Bourgoin and Corbett[12] suggested that athermal migration may proceed by successive capture of an electron and a hole, which can provide the energy to overcome a small barrier, but the path for such migration could not be determined. Semiempirical calculations[13] considered two paths, shown in Fig. 1 as TH (involving the tetrahedral and hexagonal sites) and BS (involving the bond-centered and split configurations), and concluded that the latter is far more likely to support athermal migration.

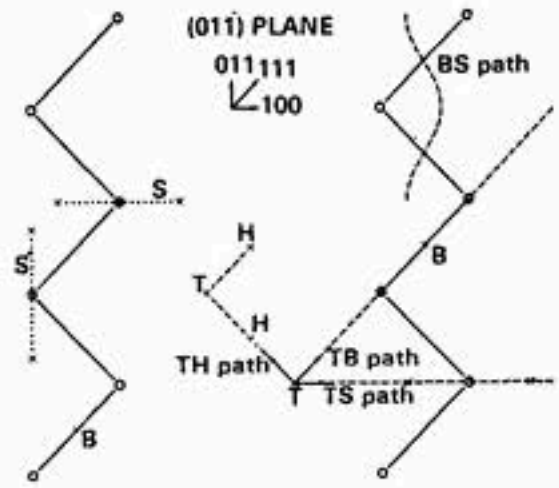

Fig. 1. Interstitial sites and paths shown schematically in one of the (110) planes. Lattice relaxations are not shown.

At high temperatures (1100-1650 K), experiments using radioactive Si isotopes as tracers found that the self-diffusion coefficient D is well described by an Arrhenius relationship of the form

$$D = D_0 \exp(-Q/kT), \tag{1}$$

with Q ranging from 4.1 to 5.1 eV.[1,2] In addition, D_0 was found to be substantially larger than corresponding values in metals.[1,2]

If there is a dominant intrinsic defect mediating self-diffusion, Eq. (1) holds and the activation energy Q is given by

$$Q = H_F + H_M, \tag{2}$$

where H_F and H_M are the formation and migration enthalpies of the defect. In addition, D_0 is proportional to $\exp(S_F+S_M)$, where S_F and S_M are the formation and migration entropies of the defect. If several defects are active, D is given by a sum of terms such as Eq.(1).

As we just saw, migration energies for vacancies and interstitials were measured at very low temperatures and found to be quite small (0-0.3 eV). These values suggest that, if either of these defects mediates self-diffusion, its formation energy must be large,[11] of order 5 eV. The formation and migration energies of vacancies and self-interstitials have not, however, been determined unambiguously in the self-diffusion temperature regime.