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Simulation of Boron Diffusion in Si Based on the Kick-Out Mechanism

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With the scaling-down of silicon devices, the simulation of diffusion profiles in silicon is essential to the fabrication of shallow junctions. Many works have already reported on the simulation of B diffusion,[1] some of which, however, rely on many parameters. These simulations lack the physical basis of diffusion, and make it difficult to apply a set of parameters determined from one diffusion condition to another condition. Therefore, a universal simulation with a reduced number of parameters which primarily contribute to B diffusion is of great importance. The purpose of this paper is to represent a description of B diffusion stripped down to the essential parameters. Based on the kick-out mechanism, B in-diffusion profiles are simulated by just three parameters, each of which has a clear physical meaning. These three parameters correspond to the fluxes of neutral boron interstitials (B_i^0), and positively charged and neutral self-interstitials (I^+ and I^0), which are taken into account as diffusion species. The physical foundation of this simulation is discussed to obtain an insight into a simulation which would be widely applicable to various B diffusion processes.

Based on the two kick-out reactions[2]: $B_i^0 \Leftrightarrow B_s^- + I^+$ and $B_i^0 \Leftrightarrow B_s^- + I^0 + h$, B in-diffusion profiles were simulated by solving the set of coupled partial differential equations using the solver ZOMBIE.[3] The local equilibrium is assumed because the kick-out reactions are regarded as fast processes. The calculated B profiles are primarily determined by the parameters: $D_s^{eff}=D_i C_i^{eq}/C_s^{eq}$, $f_{R^+}=D_{I^+}C_{I^+}^{eq}/D_i C_i^{eq}$, $f_{R^0}=D_{I^0}C_{I^0}^{eq}/D_i C_i^{eq}$, where D_s^{eff} is the effective B diffusivity, f_{R^+} or f_{R^0} is the flux ratio between I^+ or I^0 and B_i^0 species, D_x and C_x^{eq} the diffusivity and the equilibrium concentration of x.

We have satisfactorily fitted the B in-diffusion profiles,[4] as shown in Fig. 1. The deduced effective diffusivities at $p=n_i$ are very close to the reported values,[5,6] and the deduced $D_{I^+}c_{I^+}^{eq}(n_i)+D_{I^0}c_{I^0}^{eq}$ are in agreement with the self-interstitial contribution to Si self-diffusion[7] within a factor of two (c: normalized to the Si site density). In addition, the ratio of $D_{I^+}C_{I^+}^{eq}(n_i)/D_{I^0}C_{I^0}^{eq}$ is compatible with that of $C_{I^+}^{eq}(n_i)/C_{I^0}^{eq}$,[8] if we assume $D_{I^+}=D_{I^0}$. These results indicate that the three parameters used in the present simulation are physically reasonable. Due to the Fermi level effect, the concentration of I^+ is much larger than that of I^0 especially near the surface region ($f_{R^+} >> f_{R^0}$). This means that the flux of I^+ to the surface, namely f_{R^+}, primarily determines the profile shape. In the 850 and 950 °C cases, the values of f_{R^+} are smaller than one, which indicates that I^+ diffuses out slower than the B_i^0 diffuses in to become B_s^-, resulting in an I supersaturation. In the 1050 °C case, an I supersaturation also develops, but it is less significant.

B in-diffusion profiles were fitted satisfactorily using just three parameters, each of which has a clear physical meaning. This is in contrast to previous simulation studies of B in-diffusion, which rely on many parameters. We discuss why the present simulation relies on so few parameters, and its applicability to other diffusion processes from a physical viewpoint. (1) No vacancy (V) contribution is taken into account. In general, dopant diffusion is described by the substitutional-interstitial mechanism (the kick-out <via I> and the Frank-Turnbull (F-T) <via V> mechanisms) and the normal vacancy mechanism.[2,9] The fractional interstitialcy diffusion component of B has been estimated to be very close to unity.[7] *This excludes the contribution of the normal V mechanism.* In addition, due to the Fermi level effect, doping with p-type impurities increases the I equilibrium concentration, while it decreases that of V.[10] In the extrinsic region of B profiles, therefore, the V contribution via the F-T mechanism is remarkably minor, and this may generally hold for B diffusion. For the intrinsic region, the V undersaturation substantially hinders the V contribution due to the I supersaturation described above. Even if the exact local equilibrium between I and V does not hold, some amount of V undersaturation is expected. This minor V contribution retards the F-T mechanism, and consequently, *only the kick-out mechanism primarily contributes to the B in-diffusion* (both in

the extrinsic and intrinsic conditions) unless self-interstitial supersaturation is less significant, where V may contribute via the F-T mechanism to some extent, but *just in the tail region.* In contrast, no I supersaturation is observed in out-diffusion.[11,12] Therefore, to summarize the V contribution in the intrinsic region of B profiles, some V contributions via the F-T mechanism may have to be taken into account for in-diffusion without a significant I supersaturation, and for out-diffusion in general unless I supersaturation already exists in the crystal. (2) Only B_i^0, I^+, and I^0 are taken into account in this study. The physical reason is the following, and in general this may be valid for other diffusion processes: The B diffusivity is proportional to the B concentration.[5,6] This linear dependence means that the charge difference between B_s^- and a dopant interstitial is one.[13] Therefore, only B_i^0 primarily contribute to the B diffusion, and even if B_i^+ and B_i^- exist, their contributions to the B diffusion are quite minor. Concerning the charge states of self-interstitials, we take into account I^+ and I^0 based on Fair's estimation.[8] Following his estimation, the energy level of negatively charged self-interstitials I^- should be close to the conduction band, hence the I^- concentration should be very small under *p*-doping conditions. (3) Only products of D_x and C_x^{eq}, which are used as parameters, affect the calculated B profiles. This treatment is valid unless there is some interaction with other dopants, precipitation or dislocation-loop growth, *etc.* (4) The local equilibrium of the kick-out reactions is assumed because these reactions are regarded as fast processes at the temperature range and long diffusion time provided in this simulation. This allows us to ignore the rates of the kick-out reactions, but this may place some restriction on the rapid thermal annealing processes. Note, however, although some limitations are included, the present study clarifies the physical model of B diffusion, and serves as a guide for a simulation which is widely applicable to other processes such as transient enhanced diffusion of B.[8]

In summary, B in-diffusion profiles in Si were simulated based on the kick-out mechanism, taking into account neutral boron interstitials and positively charged and neutral self-interstitials as the diffusion species which primarily contribute to the diffusion. The profiles were satisfactorily fitted by just three parameters, each of which has a clear physical meaning. This study clarifies the essential parameters for B diffusion, which helps to develop a more widely applicable diffusion simulator.

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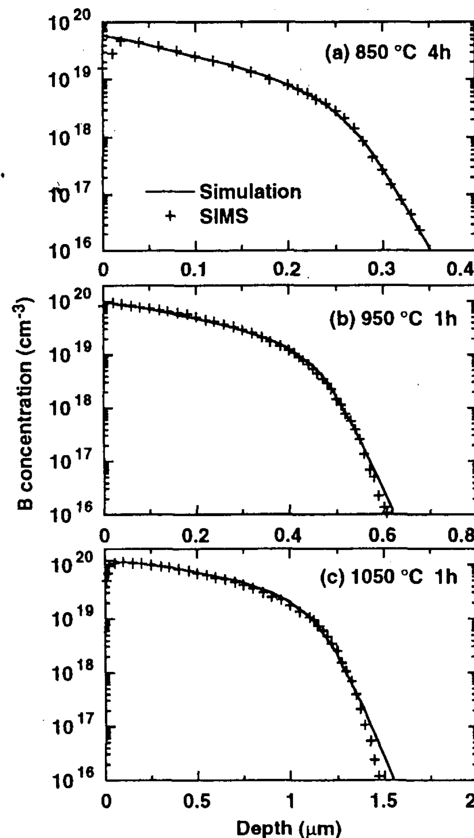

Fig. 1 Simulated and experimental[4] B in-diffusion profiles.

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