

Comments

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Vacancies, dislocations, and carbon interstitials in Si

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(Received 1 May 1986)

Song, Benson, and Watkins have recently reported injection-annealing studies of electron-irradiated float-zone-grown Si. From these, they concluded that a long-accepted identification of a deep-level transient spectroscopy level, at 0.10 eV in *n*-type Si, with the carbon interstitial is incorrect. They conclude that instead this level must belong to a complex of a vacancy with some unidentified impurity or in some self-trapped configuration. They also concluded that another long-established identification of a level at 0.44 eV with the P-vacancy complex (*E* center) is partly wrong in that a major fraction of the defects contributing to that level are a complex of a single vacancy with another unidentified impurity and perhaps also P. They further conclude that this complex exhibits a remarkable fourfold configurational metastability. Here we offer an explanation of the injection-annealing data which preserves the previous identifications of these levels. The explanation centers on analysis of the expected interaction between C interstitials and Si vacancies with small dislocation loops, which are assumed to be formed during irradiation. The same argument offers an explanation of the effects of oxidation upon dopant diffusion that does not require the presence of Si self-interstitials.

Song, Benson, and Watkins (SBW) have reported¹ deep-level transient spectroscopy (DLTS) studies of float-zone (low O content) Si that had been subjected to irradiation at room temperature by 2.5-MeV electrons in doses of either 1.5×10^{16} or 3.0×10^{16} e/cm². The samples were *n* type with 8×10^{15} P atoms/cm⁻³ and were provided with *p*⁺ contacts 0.3 μm deep by B implantation with care taken not to increase the O content. The DLTS levels were studied as a function of annealing at temperatures below 450 K with and without injection of minority carriers (holes) at a moderate level (2.5 A/cm²). Immediately after irradiation, SBW observed DLTS levels at 0.10, 0.17, 0.26, and 0.44 eV in this *n*-type Si. The level at 0.17 eV has long been associated with the complex of a single O impurity with a single Si vacancy, the *A* center; SBW do not question this identification. That at 0.44 eV has long been associated with the complex of a single substitutional P impurity with a single Si vacancy, the *E* center, while that at 0.10 eV has been associated² with the C interstitial, C_i, this is produced^{3,4} by irradiation. SBW concluded that these two identifications must be revised because (1) they found that the disappearance of the 0.10-eV level was accompanied by an increase of the other three levels plus the appearance of two additional levels, 0.23 and 0.34 eV, (2) the sum of the numbers of all defects contributing to these levels was constant, and (3) by adjusting injection temperatures it is possible to cycle strength among the 0.23-, 0.26-, 0.34-, and 0.44-eV levels reversibly. Only a

fraction (~40%) of the strength of the 0.44-eV level participates in this cycling, so SBW conclude that this fraction of the 0.44-eV level is due to some vacancy-impurity complex, *X-V*, which might include P in addition to another defect, and that this *X-V* complex has four metastable configurations, (*X-V*)_A, (*X-V*)_B, (*X-V*)_C, and (*X-V*)_D, corresponding to the 0.44-, 0.26-, 0.23-, and 0.34-eV levels, respectively. Because the disappearance of the 0.10-eV level yields a 1:1 increase in vacancy-related complexes, SBW reason that it must result either from a complex *Y-V* of a single vacancy with an unidentified impurity *Y*, or some self-trapped configuration of a single vacancy. Their data are reproduced in Figs. 1–3.

There is little question that C_i is formed during the irradiation used by SBW as a consequence of Si self-interstitials Si_i's capturing the lattice sites of substitutional C impurities, C_{Si}. There is also little doubt that the C_i has both a donor-ionization level and an acceptor-ionization level, which Kimerling, Blood, and Gibson² place 0.28 eV above the valence-band edge *E*_v and 0.12 eV below the conduction-band edge *E*_c, respectively. (C_i can be seen in electron spin resonance only when it has an unpaired spin.) Thus, the proposal that the 0.10-eV level should be ascribed to anything else begs the question of where the C_i acceptor level does lie. The DLTS spectrum shows no opportunity for an alternative assignment. Other reasons for resisting the conclusions of SBW are found in a review of the basis for the assignment of this level to

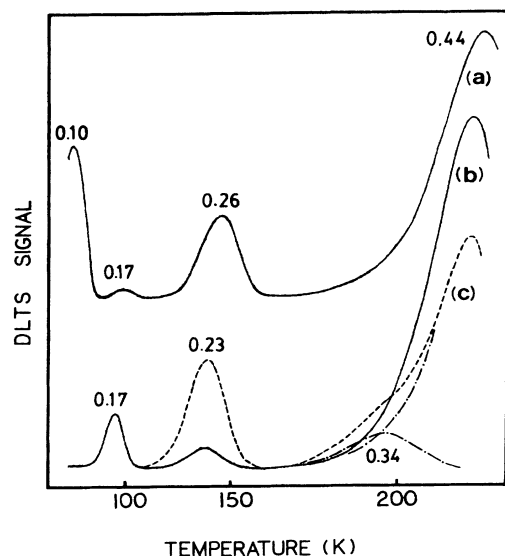


FIG. 1. DLTS spectra reported by SBW, Ref. 1, who used a 22.6 sec^{-1} rate window. (a) Immediately after room-temperature irradiation. (b) After annealing 30 min at 350 K. (c) After 240-K injection for 5 min (---). The - - - - curve shows the 0.34-eV peak after subtracting out the 0.44-eV peak.

C_i , for example in Ref. 2. It is found that the annealing rate of C_i as identified and monitored by electron paramagnetic resonance (EPR) has the same activation energy, 0.72 eV, and pre-exponential factor, $5 \times 10^7 \text{ sec}^{-1}$, as the DLTS level. Moreover, the EPR estimate of the C_i concentration is in accord with the accurate measurement

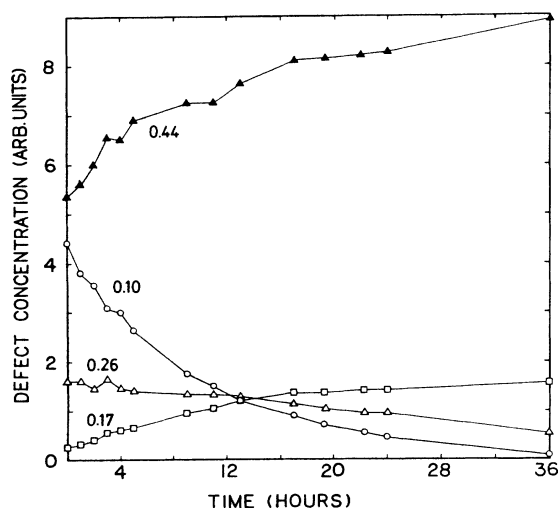


FIG. 2. Defect concentrations during isothermal annealing at 295 K following room-temperature irradiation as reported by SBW, Ref. 1. The amplitudes have been corrected (by SBW) for the presence of small peaks at 0.23 and 0.39 eV due to divacancies.

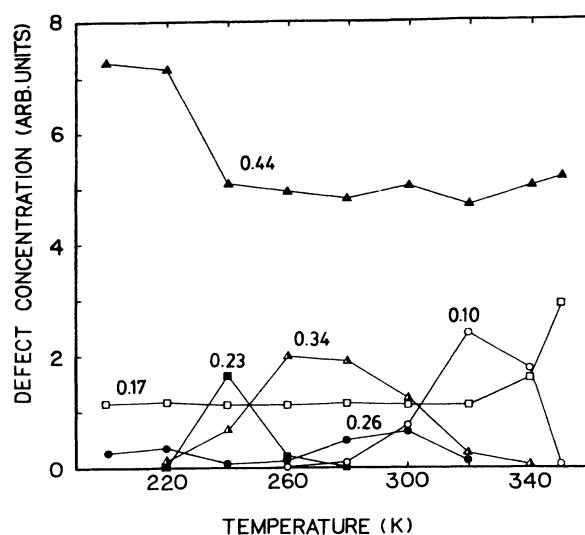


FIG. 3. Defect concentrations after injection annealing at each temperature for 5 min as reported by SBW, Ref. 1.

of this concentration by DLTS. Therefore, this author is extremely reluctant to accept the conclusions of SBW and seeks an alternative explanation of their data.

The present explanation begins with an assumption that the rather heavy irradiation used by SBW, $3 \times 10^{16} (2.5\text{-MeV } e)/\text{cm}^2$, has created a number of extrinsic, or "interstitial-type" dislocation loops in the initially dislocation-free float-zone Si. Indeed, the irradiation must initially produce V 's and Si_i 's in equal numbers, but we find [Figs. 1(a) and 2] a factor of 2 more strength in the vacancy-related DLTS peaks at 0.44, 0.26, and 0.17 eV than in the 0.10-eV peak which is here, and conventionally, ascribed to C_i 's produced from Si_i 's by the replacement reaction, $\text{Si}_i + \text{C}_{\text{Si}} \rightarrow C_i$; one must assume that about half of the original Si_i met some fate other than replacement of C_{Si} . Some of these may have reached an external surface where they can convert to being substitutional without the creation of another point defect, but it would seem that the range of the 2.5-MeV electrons is too large (several mm) that most of the lattice displacements are occurring too deep into the sample for the resulting Si_i 's to reach a surface. It seems more reasonable to assume that a large fraction of the interstitial species deficit seen in Fig. 2 is due to the formation of extrinsic dislocation loops. These are likely produced by the agglomeration of $\langle 100 \rangle$ -split Si self-di-interstitials,⁵ which are evidently much more stable than Si_i 's but sufficiently mobile at room temperature, with a migration energy of 0.6 eV, to have agglomerated in SBW's experiment. The loops are likely small and, therefore, correspondingly numerous and difficult to image in an electron microscope, because the strain field produced by an existing extrinsic loop would produce a force acting against the migration of another split di-interstitial into the loop.⁶

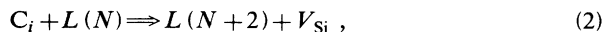
Given the assumption that small, extrinsic dislocation loops are present in SBW's samples, we make the ansatz that, because there are two atoms per unit cell in the Si

structure so that perfect dislocation loops would encompass an even number of atom sites, the enthalpy of the reaction that adds one atom to a loop containing an even number of sites differs from that of the reaction that adds an atom to a loop that contains an odd number of sites. It seems most likely that loops containing an even number of sites are more stable than loops containing an odd number of sites, but this is not necessary for the present argument. What is necessary is that a single extra interstitial, Si_i or C_i , cannot be added to a stable loop (one containing an even number of sites if that is indeed the more stable) except at the cost of some enthalpy, ΔH_0 , associated with having to accommodate an odd atom in the loop. Of course, there is also a configurational entropy associated with the accommodation of an odd atom, ΔS_0 , which would reduce the free energy of the reaction, $\Delta G_0 = \Delta H_0 - T\Delta S_0$, at any temperature T . As long as the loop is small and T is low so that there would only be one odd atom at a time, ΔS_0 might be estimated as $\Delta S_0 = k \ln N_p$, where k is Boltzmann's constant and N_p is the number of sites on the perimeter of the loop. We might approximate N_p as $(N/\pi)^{0.5}$, where N is the number of sites in the loop. As long as N and T are both small enough that $\Delta G_0 \gg 0$, the loops will have a definite tendency not to accept either a single interstitial or a single vacancy, either of which would require the accommodation of an odd atom. (There would be no hindrance of the incorporation of divacancies or di-interstitials beyond that produced by the strain field.⁶) Note that when N and T are large enough that $\Delta G_0 < 0$, the loop will exhibit no tendency to prefer either an odd or an even number of sites; the free energy will be minimized with configurations that have several odd atoms about the loops. (This perimeter roughening of the loops is analogous to the surface roughening of crystal facets that occurs at sufficient temperature.)

Given this ansatz and the assumption that small dislocation loops are present, let us now consider the interaction of C_i with a stable dislocation loop containing (an even number) N sites, which we denote $L(N)$. The reaction



would release an enthalpy $\Delta H(C_i) - \Delta H_0$, while the reaction



in which the C takes an atom from the lattice into the loop with it so that the resultant loop can also be perfect, and so that a single vacancy is emitted, releases an enthalpy, $\Delta H(C_i) - H(V_{Si})$. Provided that

$$\Delta H_0 > \Delta H(V_{Si}) \quad (3)$$

Reaction (2) will predominate over Reaction (1) and we will expect the concentration of vacancy-related defect complexes to increase in 1:1 relation to the decrease in C_i , the defect responsible for the 0.10-eV DLTS level, as was observed by SBW.

A rigorous quantitative justification for inequality (3) beyond this author's present capacity, and would seem to

be beyond the scope of the present Comment. However, the remainder of this paper provides that which the author considers a convincing empirical case—that inequality (3) in fact holds for Si. One can note that the common observation of partial dislocations in Si with the stacking faults between them⁶ seems to imply that the stacking-fault energy alone is not large enough to account for Eq. (3). The likely source of the major contribution of energy to H_0 comes from the structure of the core of the dislocation, which runs around the perimeter of the loop.

Let us now consider other properties of the 0.10-eV level. Both SBW and Ref. 2 note that the small pre-exponential factor $5 \times 10^7 \text{ sec}^{-1}$ in its annealing rate suggests that the defect migrates as a single entity, though about 10^5 sites before its reacts with something else. This is consistent with the identification of the defect as C_i and the assumption that its fate is to join a dislocation loop. If it were a $Y-V$ complex it would have to be rather tightly bound at the third-nearest-neighbor site, so that the complex would reform after it had separated during the migration process 10^5 times. (Such behavior is exhibited by the divacancy in Si,⁷⁻⁹ but is rather unusual.) Moreover, the disappearance of the 0.10-eV level would then be ascribed to the separation of the complex to isolated Y plus the V_{Si} ; one would expect to find the isolated Y creating a level in the DLTS spectrum, but there is no extra level to assign.

Another remarkable property of the 0.10-eV level observed by SBW is that after it has disappeared it can be regenerated by injection annealing with $T=320 \text{ K}$ (Fig. 3). No explanation has been given as to why the $Y-V$ complex should reform under these conditions. As for the present explanation, we note that the values of $\Delta H(C_i)$ and $\Delta H(V_{Si})$ appropriate to Eq. (3) are affected by the position and splitting of (quasi-) Fermi levels. In n -type material in the absence of hole injection, one would have

$$\begin{aligned} \Delta H(V_{Si}) = & \Delta H_f(V^0) - [E_F - H_i(V^-)] \\ & - [E_F - H_i(V^{2-})] \end{aligned} \quad (4)$$

where E_F is the Fermi level, $\Delta H_f(V^0)$ is the enthalpy of formation of the neutral vacancy, which is^{9,10} $2.4 \pm 0.2 \text{ eV}$, and $H_i(V^-)$ and $H_i(V^{2-})$ are the enthalpies of the ionization levels of V_{Si} to the first- and second-acceptor states.¹¹ We note that n -type doping makes Reaction (2) more favorable because it reduces the enthalpy cost of V^{2-} and V^- . The corresponding reduction in enthalpy cost for C_i is negligible because its acceptor level is no more than 0.10 eV below the conduction-band edge. The injection of holes will lower E_F and thereby reduce the advantage given by Eq. (4) to vacancies over C_i 's. For high levels of injection, the limit of this change would be $2E_c - H_i(V^-) - H_i(V^{2-})$ or about 0.9 eV. Evidently, the 2.5-A/cm^2 injection level used by SBW must be combined with the thermal effect of 320 K to reverse the sign of the free-energy difference corresponding to Eq. (3), so that the reverse of Reaction (2) will occur and generate C_i 's at the expense of vacancy complexes. (Injection annealing below 280 K does not seem to have this effect.) The thermal effects should be a combination of the entropy factor $T\Delta S_0$, for which N probably increases with T , and a

difference in formation entropy between C_i and V_{Si} . While the author is not aware of any empirical value for the entropy of formation of C_i , it seems likely it is greater than that for V_{Si} .

Consider now the interaction of V_{Si} 's with the dislocation loops. These also will be inhibited from joining the loops as long as they are small enough and as long as T is low enough that Eq. (3) is obeyed because they too would change the number of sites involved in a loop from even to odd. However, V_{Si} 's are attracted toward the loop in directions where it produces tensile strain⁶ with a climb force per unit length of dislocation

$$dK_z/ds = \frac{b^2 G}{2\pi(1-\nu)} \frac{z(3x^2+z^2)}{(x^2+z^2)^2} \quad (5)$$

for the case of an edge dislocation with Burgers vector b in the x direction and core segment ds in the $-y$ direction. Here $G \sim 8 \times 10^{11}$ dynes/cm² for Si is the shear modulus and $\nu \sim \frac{1}{3}$ is Poisson's ratio. Of course, Eq. (5) diverges at distances $r = (x^2+z^2)^{0.5}$ too close to the core and is not applicable for $r < r_0 \sim 1$ nm, the boundary of validity of the linear elastic theory from which it is derived. Evaluating this climb force for V_{Si} 's at r_0 one finds it is about 4×10^3 dynes/cm or 1 eV/bond length. This is of the same order as the Coulomb force between V_{Si}^- and P_{Si}^+ that binds the E center.

Therefore, we must expect any E center that finds itself near one of these dislocation loops to tend to migrate toward the loop along directions of increasing tensile strain. Indeed, we see in Fig. 2 that about 40% of the 0.44-eV structure that is present after the first annealing step is derived from the 0.10-eV structure that is removed in that step. Thus, in terms of the present (conventional) interpretation of these peaks, 40% of the E centers present at this point came from the V_{Si} 's that were emitted when the C_i 's joined the loops (presumably at the dislocation cores on their perimeters). As these V_{Si}^- 's emerged from the core region, they were attracted back toward the loop by the strain field but also toward P_{Si}^+ 's, which were present not too far from the loop in the doped Si, by the Coulomb field. The net (free) energy was reduced as the V_{Si} 's caused the P_{Si} to migrate toward the loop along the favorable directions defined by the strain field. We must assume this was the dominant fate of the V_{Si} 's that were emitted from the loops. From Fig. 2, the rough estimate that 80% of these V_{Si} 's met this fate is made by noting that 80% of the original 0.10-eV strength approximates the 40% of the final 0.44-eV strength that is derived from disappearance of the former. The remaining 20% of the V_{Si} evidently make A centers with the oxygen present.

However, in order to continue to move the P_{Si} in this direction, the V_{Si} must move around the sixfold ring of the Si structure in that direction. When the V_{Si} reaches the r_0 boundary of the dislocation, i.e., the loop perimeter, it will not be able to continue, because it cannot join the loop, and cannot move the P_{Si} any closer. The situation is illustrated in Fig. 4 for a reasonable assumption of the lattice geometry beyond r_0 . (Very little is known about the core structure so we do not speculate upon it.) We see that there are two metastable positions for the P_{Si} , one (a)

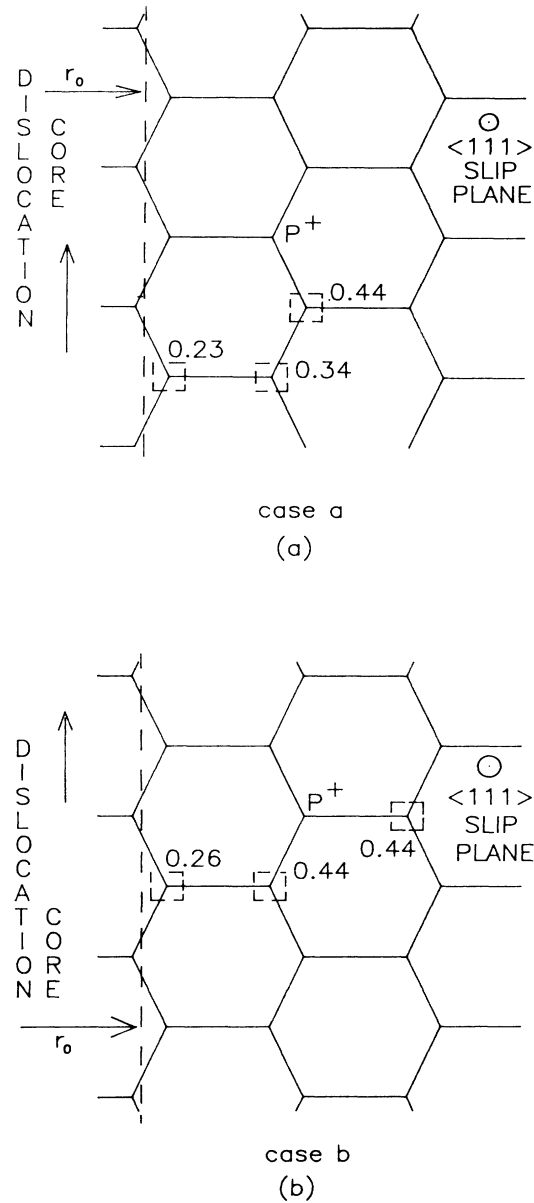


FIG. 4. Si lattice just outside boundary of the dislocation core, ~ 1 nm from core center, showing metastable configurations of a P_{Si} - V_{Si} pair. In case (a), the P_{Si} is as near to the core boundary as it can get, ~ 0.25 nm. The V_{Si} has one metastable position across the ring, where it is on the core boundary—so as to minimize elastic energy, and another as second-nearest neighbor to the P_{Si} , where it has lower electrostatic energy due to Coulomb binding with the P donor. These positions are here associated with the 0.23- and 0.34-eV levels observed by SBW, Ref. 1. In case (b) the P_{Si} is somewhat further from the core boundary, ~ 0.33 nm. In this case the V_{Si} can take a position on the core boundary, to minimize the elastic energy and yet be a second-nearest neighbor of the P_{Si} , so as to benefit from the Coulomb attraction. This configuration is here assigned to the 0.26-eV level of SBW. It is here assumed that any configuration for which the P_{Si} and V_{Si} are nearest neighbors give rise to a DLTS level at 0.44 eV below the conduction-band edge, as is found for E centers in the bulk of the sample.

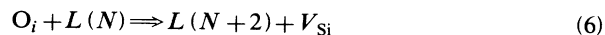
about 0.25 nm from the core boundary and the other (b) about 0.33 nm from the boundary. In case (b) the V_{Si} has metastable positions either at first-nearest-neighbor positions to the P_{Si} , where the Coulomb energy is maximized, or at two sites on the core boundary, which are second-nearest neighbors to the P_{Si} , where the strain energy would be minimized at the cost of some Coulomb energy. For case (a) we note that there is no way that the V_{Si} can reach the site on the core boundary directly beneath the P_{Si} ; the other nearest-neighbor sites all place the V_{Si} further than 0.25 nm from the core boundary and therefore probably have little stability. The more stable configurations for case (b) would seem to be those that have the V_{Si} on the core boundary across the ring from P_{Si} and as second-nearest neighbor to P_{Si} where it is 0.25 nm from the core boundary. If we now assume that the DLTS level of these complexes is primarily affected by the spacing between P_{Si} and V_{Si} , and secondarily affected by the strain field of the dislocation outside r_0 , we can conclude the following: all configurations for which V_{Si} is the nearest neighbor give rise to a level 0.44 eV below the conduction-band edge; configurations with V_{Si} as second-nearest neighbor give the level at 0.34 eV in case (a), where the strain is less, and the level at 0.26 eV in case (b) where the strain is greater; and the configuration of case (a) with V_{Si} across the ring and in the region of maximal strain on the core boundary gives the 0.23-eV level. Of course, these metastable configurations of the E center next to the dislocation loop can cycle amongst each other by migrating the V_{Si} around the ring with the P_{Si} . This should be expected to occur under hole injection, which would turn on and off the Coulomb attraction that balances the elastic force trying to move the V_{Si} away from the P_{Si} and toward the core boundary.

Those E centers which were not created near a loop and do not encounter a dislocation loop during their limited migration in the course of the experiment remain in relatively strain-free regions of the sample and will only be stable with the V_{Si} nearest neighbor to the P_{Si} ; these will give only the 0.44-eV level and will not cycle. Thus, the division between the 60% of E centers which do not cycle and the 40% that do is just a consequence of the probability that a given E center is near a dislocation loop under the conditions of the SBW experiment. This in turn is a function of the number of C_i 's initially present and the probability that the emitted V_{Si} finds a P_{Si} near the loop.

We see that it is possible to account for all the remarkable features of injection annealing reported by SBW in a natural way without having to reject long standing and very reasonable assignments of DLTS levels to EPR identified C_i and $P_{\text{Si}}-V_{\text{Si}}$ pairs. This allows us to avoid the problem of finding a new level for C_i , which must be there, and new levels for the presumed Y_{Si} and X_{Si} , where X and Y are impurities other than C, O, and P, for which no other evidence has been found in very pure Si.

A consequence of this analysis is that we must expect reactions similar to (2) in other cases where small dislocation loops are punched out in semiconductors with the Si or GaAs lattice structure. An important case occurs during the precipitation of SiO_2 in Si. It has been observed that oxidation with the consequent punching-out of dislo-

cation loops can either increase or decrease the rate of dopant diffusion depending closely on the situation.¹² The loops grow as O_i 's that were grown into Czochralski Si precipitate to form SiO_2 and swell to produce strains beyond the elastic limit of the host lattice. The fact that dopant diffusion can be both increased and decreased by this process has caused many to postulate that Si self-interstitials, Si_i 's, as well as V_{Si} 's, mediate the diffusion of these impurities, whereas otherwise there is very little evidence for any participation of Si_i 's.^{10,12} We now see that where the loops are small, the reaction



is expected and should increase the rate of dopant diffusion through purely vacancy-mediate processes. When the loops are so large and T so high that $G_0 < 0$, we may expect these loops to act as vacancy sinks and reduce the local V_{Si} concentration below its equilibrium value so that dopant diffusion will be suppressed.⁶ Of course, one should keep in mind long standing arguments that dislocations are always both sinks and sources for both vacancies and interstitials because they always produce regions of both tensile and compressive strain.^{13,14} [Note that Eq. (5) changes sign on going from $+z$ to $-z$.]

Further evidence that dislocation climb in Si does indeed inject V_{Si} 's into the bulk of the sample is found in the positron annihilation study of plastic deformation of Si made¹⁵ by Dannefaer *et al.* They plastically deformed low-O, float-zone-grown Si at 800 C in a vacuum. They observed an introduction of free volume to be concomitant with this process by making positron lifetime studies over a range of temperatures and annealing conditions. Two components of the exponential decay of the positrons were resolved. The longer component, with a characteristic time of 1.8 nsec, was evidently related to the cores of the dislocations that were induced by the deformation because it did not anneal out until the dislocations annealed out. The large voids associated with such a long lifetime might be associated with the cores of the dislocations, particularly where two dislocations intersect. However, it seems more likely that such large voids (about 2 nm in diameter) result from accumulation of vacancies at particular sites along the dislocations. The shorter lifetime, 734 psec, is characteristic of a $6V_{\text{Si}}$ complex and was observed to anneal out well below the annealing of the dislocations. It is most likely that these clusters of vacancies formed from single V_{Si} 's, or small clusters of vacancies, that were evidently injected by the deformation process. (The samples were cooled to room temperature after deformation and cut to form positron samples.) While deformation implies the nucleation and glide (i.e., conservation motion) of dislocations, it is generally accompanied by climb (i.e., dislocation motion via emission or absorption of vacancies or of interstitials). As no vacancies or other voids could be detected in these samples before the deformation, one must conclude that deformation induces free volume, most likely in the form of vacancies, into Si. Such a deformation process must, by definition, include a component of climb to correspond to this nonconservation of lattice sites.

Of course, both the accumulation of C_i 's at the dislocation loops in the SBW experiment (according to the present interpretation) and the deformation of Si concomitant with the formation of SiO_2 precipitates are examples of dislocation climb. There seems to be every reason to

believe that these climb processes will also inject vacancies into the bulk of a Si sample. Indeed, Dannefaer and Kerr will shortly publish positron studies¹⁶ of the initial phase of the formation of oxide precipitates in Si indicating that vacancies are produced in that process.

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