LATTICE DILATATION OF BORON IN SILICON

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Recent data on laser-annealed, boron-implanted silicon are analysed, and the results compared with earlier experiments and simple theory. Each substitutional boron decreases the total volume by about 90% of the volume per silicon atom in the perfect crystal.

One notable effect of laser annealing is that it can produce silicon in which virtually all the donors or acceptors are present substitutionally, even at high doping levels. The usual complications of precipitates can be avoided. Recently Larson et al. [1] measured the change in lattice parameter of a layer of boron-doped silicon which had been laser-annealed. The published data allow one to estimate the strain field of the dopant, and to compare the results with volume expansion data from conventionally prepared samples [2–5].

The experimental arrangements were different in the two types of experiment. The earlier workers' results are for crystals doped roughly uniformly, and can be expressed in terms of a volume change ΔV per dopant atom; usually this is given in units of the volume Ω per atom in the perfect host. Larson et al. implanted only a thin layer before laser-annealing. The remainder of the crystal acted as a substrate which prevented lateral strain, and this constraint shows up in the lattice strain caused by the dopants. When the crystal surface is (001), the resulting strained region has a finite value of $\epsilon \equiv e_{zz}$, with negligible (ideally zero) values of the other strain components. In this note we relate e_{zz} to $\Delta V/\Omega$, and compare the data of refs. [1–4] with each other and with simple models.

The value of ϵ can be deduced using the Betti Reciprocity Theorem [6,7] with a straightforward generalisation. The calculation proceeds in two steps. First, one calculates the dimension change δ normal to the surface. Each defect may be represented by a set of defect forces such as acting $\boldsymbol{F}_i$ acting at points $(\boldsymbol{R}_i + \boldsymbol{R}_0)$ relative to a defect at $\boldsymbol{R}_0$. We shall assume that, for all but a negligible fraction of the dopants, the defect forces act entirely within the crystal. A key quantity is the virial $G_{\alpha\beta}$, defined by:

$$G_{\alpha\beta} = \sum_i F_{i\alpha} R_{i\beta} , \tag{1}$$

where i labels the sites near a single dopant at which the defect forces act. If there are ρ_A defects per unit area of surface and if e_{zz} alone is finite:

$$\delta = \rho_A G_{zz}/c_{11} , \tag{2}$$

where the elastic constants are c_{ij}. The second step is to assume the dopant atoms are distributed roughly uniformly over a depth D. The volume density of dopants is then

$$\rho = \rho_A/D , \tag{3}$$

and the contribution to the strain ϵ per defect is

$$\epsilon \equiv \delta/\rho D = G_{zz}/c_{11} . \tag{4}$$

This can be compared with previous results for the volume change:

$$\Delta V/\Omega = (G_{xx} + G_{yy} + G_{zz})/(c_{11} + 2c_{12}) . \tag{5}$$

If the dopants are all at sites of at least tetrahedral symmetry, so $G_{xx} = G_{yy} = G_{zz}$, then:

$$\epsilon = (\Delta V/\Omega)(3c_{11}/(c_{11} + 2c_{12})) ,$$

$$(\Delta V/\Omega) = \epsilon \cdot (c_{11} + 2c_{12})/3c_{11} . \tag{6}$$

The various experimental results can be summarised:

$$\left.\begin{array}{l} \Delta V/\Omega = -0.91\ [1] \\ \qquad\quad +0.07\ [2] \\ \qquad\quad -0.34\ [3] \\ \qquad\quad -0.85\ [4] \\ \qquad\quad -0.68\ [5] \end{array}\right\} \text{experiment},$$

$$\qquad\quad -0.71 \qquad \text{simple theory}.$$

The theory value uses the approximation for simple substitutional donors or acceptors that ΔV is the same as $(\Omega_D - \Omega_H)$, where Ω_H is the volume per atom of the group IV host and Ω_D the volume per atom of the group IV element in the same row of the periodic table as the dopant.

The conclusions are that the laser-anneal results, the measurements of ref. [4] and the simple theory all agree reasonably well, whereas the earlier data [2,3] appear to show problems from precipitate formation. Further since the experiments described were done at very different concentrations (5×10^{18} cm^{-3} in ref. [4]; 0.5×10^{21} and 1.25×10^{21} cm^{-3} in ref. [1]), the results imply that the virial (1) depends little on carrier density. Thus the virial does not contain any significant term from the weakly bound electron or hole of the shallow donor. This agrees with previous estimates ([8] § 23.4.2). Likewise, the small concentration-dependent effects on the c_{ij} [9] seem to have little effect on the values of ΔV.

References

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