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Defects in Semiconductors

A TENTATIVE IDENTIFICATION OF THE NATURE OF {113} STACKING FAULTS IN Si - MODEL AND EXPERIMENT

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ABSTRACT

An atomic model with fully bonded interstitial atoms is proposed for the {113} stacking faults (SF). It is shown that the development of the {113} habit plane is a result of minimizing bond length changes. The fault may be represented by a $\frac{1}{11}$<113> partial dislocation, and a $\frac{3}{22}$<332> partial will facilitate an unfaulting reaction to result in a $\frac{1}{2}$<110> 90° edge dislocation. Lattice images were obtained for a {113} SF which showed that the model is essentially correct.

INTRODUCTION

In high energy (1000keV) electon damaged thin samples of Si(Ge),[1-4] and in thermally annealed, ion-damaged Si crystals,[5,6] there exists a peculiar class of defects not found in metals: the so-called rod-like defects and {113} stacking faults (SF). In our previous papers,[7,8] it was shown that a better understanding of the nature of rod-like defects has now been obtained. The purpose of this paper is to show that for {113}SF it is also possible to obtain a model with all four coordinated Si(Ge) atoms and our preliminary experimental results tends to support this model.

THE MODEL

From observation of electron irradiated Si(Ge) thin samples in situ in high voltage electron microscopes, it is established that the {113}SF are characterized by: (1) a prominent growth in a <110> direction and a minor growth in a <332> direction, so that the habit plane of the defect is a {113}.[1-4] (2) The SF unfaults by a shear, which results in a unique 1/2 <110> interstitial loop.[3] (3) The SF is extrinsic,[1-4] and (4) the matrix crystal is displaced by $\sim \frac{1}{25}$<116>.[2] The only reported model of this defect invokes the use of interstitial atoms each with three dangling bonds and the bonds of matrix crystal atoms on either side of the fault plane are stretched by 35-48%.[3] We view this model as highly unlikely because it implies a high energy situation. Here we propose an atomic model for the {113} SF with all 4-coordinated atoms satisfying the above listed properties. Fig. 1(a) shows the first step of the modeling: two neighboring rows of $[\bar{1}11]$ bonds of a row of 6-membered rings are cut and the cell is pulled apart so as to insert a row of interstitial atoms. The formation of new bonds results in two conjugate pairs of 5-7 membered rings - this is just the IDC of the 90° edge dislocation.[7] There is no dangling bond for the inserted atoms not at the two ends of the defect. The two end atoms each have a dangling bond and the defect is easy to grow in the $[\bar{1}10]$ direction. The defect can now go into climb motion in a direction lying in the $(\bar{1}10)$ plane. As a result of not allowing the presence of any dangling bonds and minimizing atomic stresses, i.e., bond stretches, only two configurations may be derived, one is the 90° edge dipole due to climb,[7] the other is the one shown in Fig. 1b, for which the climb direction is $\pm$ [332] and the habit plane of the

defect is $(\bar{1}\bar{1}3)$. The (minor) growth in <332> direction is due to climb and a minimization of bond stretches, and in Fig. 1(b) every bond length is not changed by more than 5% of the normal Si atom bond length. Because the total number of interstitial atoms in the fault layer equals that of a monolayer of {113} plane, a Burgers vector of $\frac{1}{11}[11\bar{3}]$ may be defined for its bounding partial dislocation, and unfaulting reaction may be accomplished by the nucleation of a $\frac{3}{22}[332]$ partial. The 3/22 [322] partial sweeps through the fault, with bounding rearrangement shown in Fig. 1(c), to arrive at a $\frac{1}{2}[110]$ 90° edge dislocation dipole, see Fig. 1(d). Thus this $(\bar{1}13)$SF satisfies the above discussed characteristics (1) to (3). However, the matrix crystal displacement is now $\sim \frac{1}{5}[\bar{1}\bar{1}1]$ instead of $\sim \frac{1}{25}<116>$. To rectify this situation, we consider the segregation of C and O interstitials to the defect as Aseev et al has observed.[16] If 50% of Si self-interstitials is replaced by C, and an equal number of O interstitials is segregated to the bond centered positions of the 7-membered rings, we obtain Fig. 2 which has a matrix crystal displacement of $\sim\frac{1}{25}[\bar{1}16]$. Notice that the covalent radii of Si, C and O are respectively 1.17Å, 0.77Å and 0.66Å, we see no severe bond length changes are involved. The incorporation of C and O do not effect the unfaulting reaction, but after unfaulting C and O will tend to de-segregate and they may form small ppt.-like defects. Salisbury and Loretto[3] and Aseev et al[4] have observed such phenomena.

EXPERIMENT

For our experiment, p-type20Ωcm, <001> oriented CZ Si wafers were implanted by 50keV H^+ ions to a dose of $4x10^{16}/cm^2$ at a substrate temperature of 575°C. Weak beam imaging of these samples showed that {113} SF 40Å wide and up to 1μ long were produced in a depth of 2500Å to 5000Å below the sample surface.[6] <110> cross-sectional sample were made from these wafers and imaged in a Siemens 102 electron microscope in the lattice imaging mode by including seven beams, 000, $\pm\bar{1}11,\pm111,\pm002$ in the objective aperture.

Fig. 3(a) shows the lattice image of a {113} F. Two things are immediatedly clear: (1). The habit plane is $(\bar{1}\bar{1}3)$, (2). When measured against a perfect Si crystal lattice drawn to scale, Fig. 3(b), it is found that the matrix crystal displacement is $\sim \frac{1}{25}[11\bar{6}]$. This is the first direct measurement of the displacement and the second accurate measurement using any method.[2]

The images of the atomic columns on the fault plane are generally hard to see. However, at the lower left end it is possible to analyze the finge patterns, and draw the atomic structures, Fig. 4(a). For this tiny patch it is seen that this is consistent with our model. Fig. 4(b) shows a calculated micrograph for comparison purposes. The micrograph contains regions where a direct comparison with our model is not possible probably because the fault is jogged.

CONCLUSION

A model that meets all the essential characteristics of the {113} SF is obtained with fully bonded interstitial atoms, and on a preliminary basis, is in good agreement with the experimental results obtained.

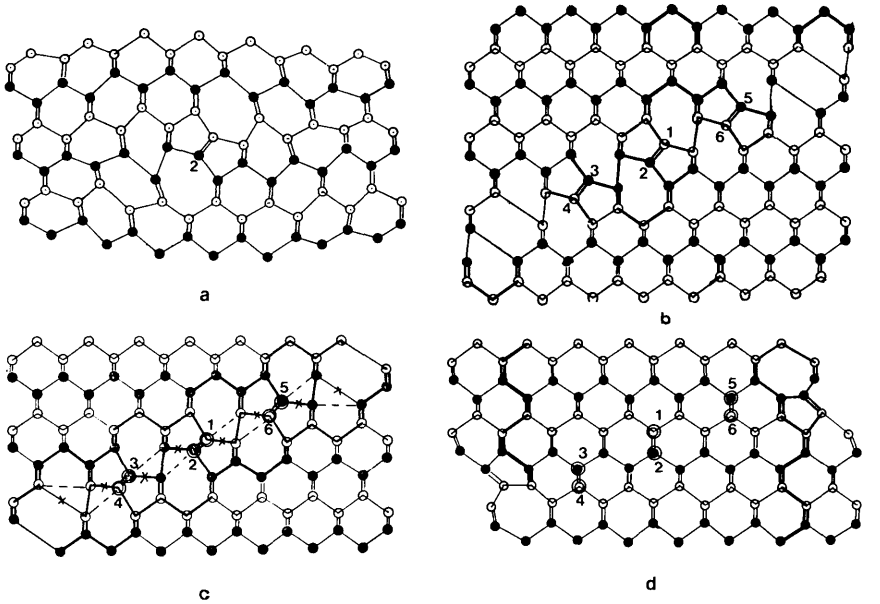


Fig. 1. The $(\bar{1}\bar{1}3)$ SF model. (a). The extrinsic 90° edge dislocation IDC, (b). The $(\bar{1}\bar{1}3)$ SF with a matrix displacement of $1/5[\bar{1}\bar{1}1]$, (c). Bond rearrangement during unfaulting by a $3/22[332]$ partial dislocation, and (d). The resultant extrinsic 90° edge dislocation dipole.

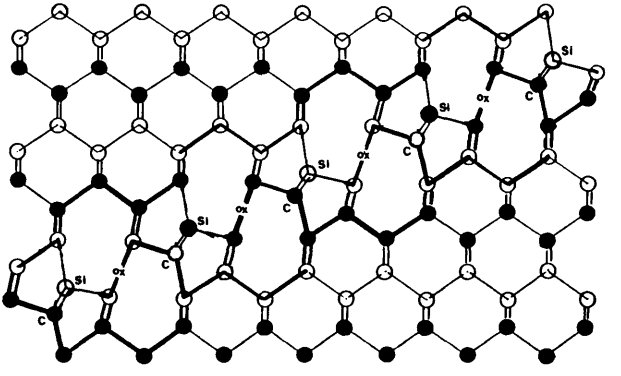
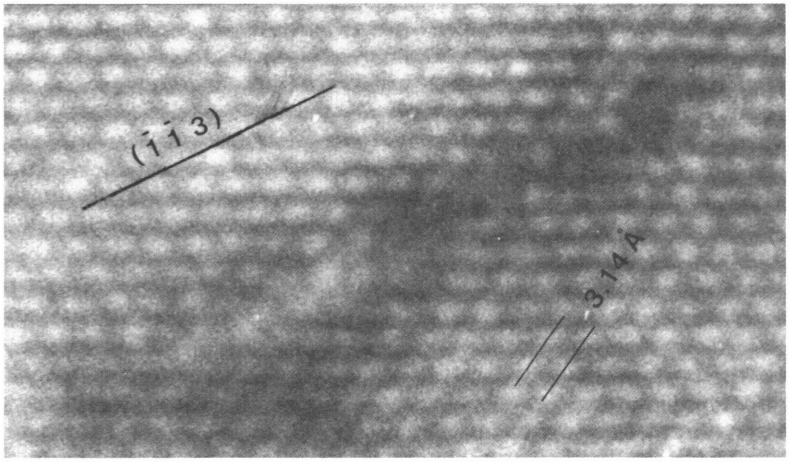
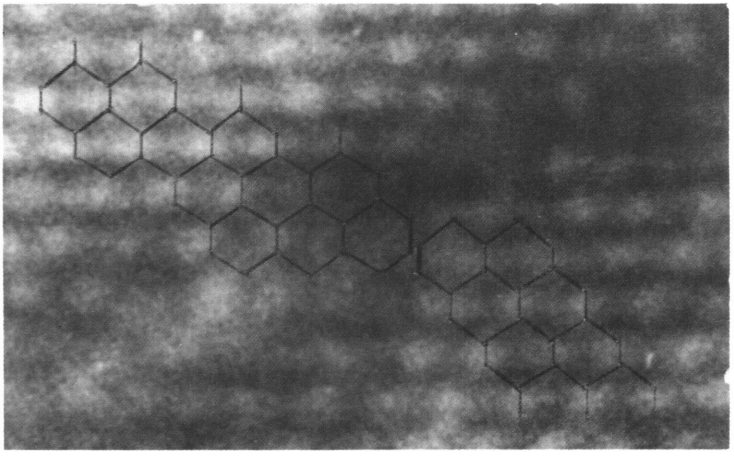


Fig. 2. The $(\bar{1}\bar{1}3)$ SF model incorporated C and O to yield a matrix crystal displacement of $1/25[11\bar{6}]$.

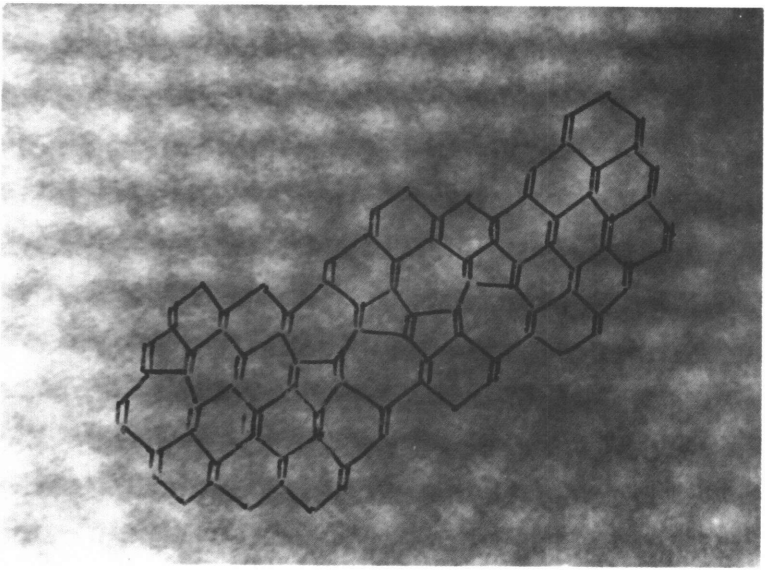


a

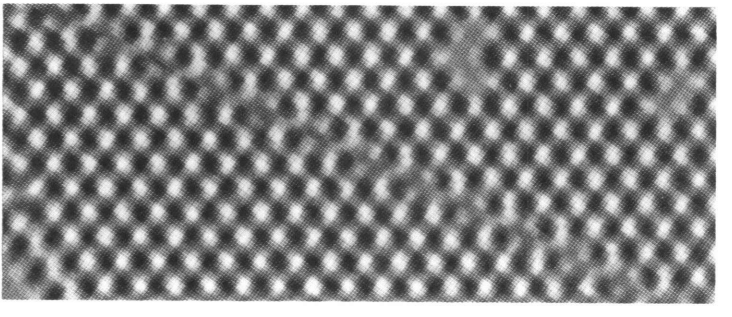


b

Fig. 3. An experimental (113) SF. (a). The lattice image, (b). An enlarged portion of (a) with two lattices drawn in on either side of the SF. The two lattices has a relative displacemant of $1/25[11\bar{6}]$. This shows that the matrix displacemant is $\sim 1/25[11\bar{6}]$.



a



b

Fig. 4. (a). An enlarged view of the lower left part of the SF in figure 3(a) with possible structure drawn in. This shows that at least some part of the SF is consistent with our proposed model, (b). Calculated image of the SF with CTF=1.

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