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Activities of dislocations in heavily impurity-doped Si

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Abstract. The dynamic behaviour of dislocations in heavily impurity-doped Si crystals is investigated. Suppression of the generation of dislocations from a surface scratch is found for Si doped with B and P to a concentration higher than 1×10^{19} cm^{-3} and the critical stress for dislocation generation increases with B and P concentration which is interpreted in terms of dislocation locking due to impurity segregation. The velocity of dislocations in B- and P-doped crystals increases with increasing B and P concentration, respectively.

1. Introduction

The interaction between dislocations and impurities in semiconductors has two interesting aspects. One is the effect of dislocations on the spatial distribution of impurities in a crystal. The other is the effect of impurities on the dynamic activity of dislocations. In silicon crystals, oxygen and nitrogen impurities are known to have a strong effect on dislocation immobilization due to preferential segregation [1]. Donor impurities, such as phosphorus, in addition to their strong immobilization effect on dislocations, enhance the velocity of dislocations [1, 2]. Contrarily, no appreciable effect on either the immobilization or the mobility of dislocations caused by an acceptor impurity is known [1, 2]. However, knowledge on the dynamic activity of dislocations in heavily impurity-doped Si is very limited. In current advanced technology, Si crystals heavily doped with electrically active impurities are used as the substrate material for the epitaxial growth of clean wafers without grown-in defects. Dislocation generation within large-diameter Si wafers becomes a serious problem because of their intrinsic weight. Thus, it is very important to clarify the dislocation activity in such heavily impurity-doped crystals from both the practical and fundamental viewpoints. Recently, dislocation-free Si crystals have been successfully grown by the Czochralski technique, without the Dash necking process, with high levels of doping with boron impurity [3].

This paper reports on the dynamic behaviour of dislocations in Si crystals doped with boron (B) and phosphorus (P) to various concentrations up to 2.5×10^{20} cm^{-3}.

2. Experimental procedure

Specimens were prepared from dislocation-free Czochralski-grown (CZ) Si crystals doped with various B and P concentrations together with undoped CZ-Si and float-zone-grown (FZ-grown) Si crystals doped with B and P impurities for comparison. Specimens were sectioned into rectangular shapes, approximately $2 \times 3 \times 15$ mm^3, with the long axis along the direction $[1\bar{1}0]$ and side surfaces parallel to (111) and $(11\bar{2})$. Scratches were made on the chemically finished (111) and $(\bar{1}\bar{1}\bar{1})$ surfaces of the specimen along the $[1\bar{1}0]$ direction at room temperature with a diamond stylus. Such scratches serve as preferential generation centres for dislocations when stressing the specimen. The specimen was stressed at elevated temperature by means of three-point bending in a vacuum. The bending axis was parallel to [11$\bar{2}$]. The generation and motion of dislocations from the scratch were detected by observing the etch pits developed by Sirtl etchant [4] at 20 °C. The geometry of the specimens as well as the details of the experimental procedure are described in a previous article [5].

3. Results and discussion

The generation of dislocations from a scratch under various stresses has been investigated. The distance travelled by the leading 60° dislocation in an array of dislocations that are generated from a scratch during a 10 min stress pulse at 800 °C is plotted against the resolved shear stress in figure 1 for undoped FZ-Si, undoped CZ-Si, and B-doped CZ-Si. It is seen that there is a critical stress for the generation of 60° dislocations in undoped and B-doped CZ-Si. The magnitude of the critical stress can be as high as ≈7 MPa and 15 MPa in undoped and B-doped CZ-Si, respectively. No appreciable critical stress is measured for dislocation generation in undoped FZ-Si. Once the stress exceeds the critical stress for generation, the travel distances in the undoped and B-doped CZ-Si increase rapidly with stress. In such a case, the relationship of the travel distance and the stress usually shows a break at some high stress, beyond which the travel distance increases with stress at approximately the same rate as found for undoped FZ-Si. For high stress, the relationship of the travel distance and the stress for undoped CZ-Si coincides with that of undoped FZ-Si. Contrarily, the travel distance in B-doped CZ-Si is larger than that in undoped FZ-Si, which means that there is a velocity enhancement caused by B doping as discussed later.

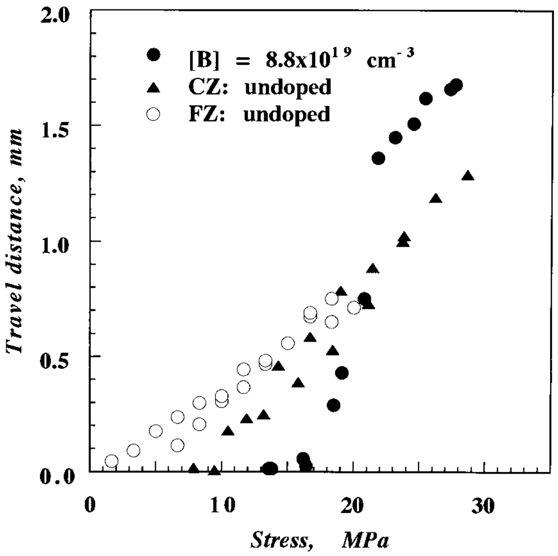


Figure 1. Travel distance of leading 60° dislocations generated from a scratch during a 10 min stress pulse at 800 °C plotted against stress for various Si crystals.

Figure 2 shows the dependence of the critical stress for dislocation generation on the concentration of B and P impurities. The critical stress increases dramatically when the B and P concentrations exceed 1×10^{19} cm^{-3}, which means that B and P concentrations

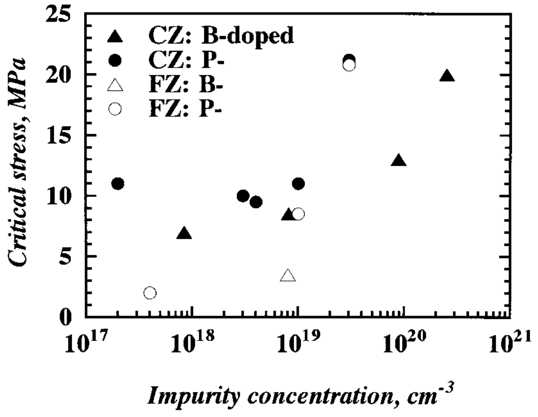
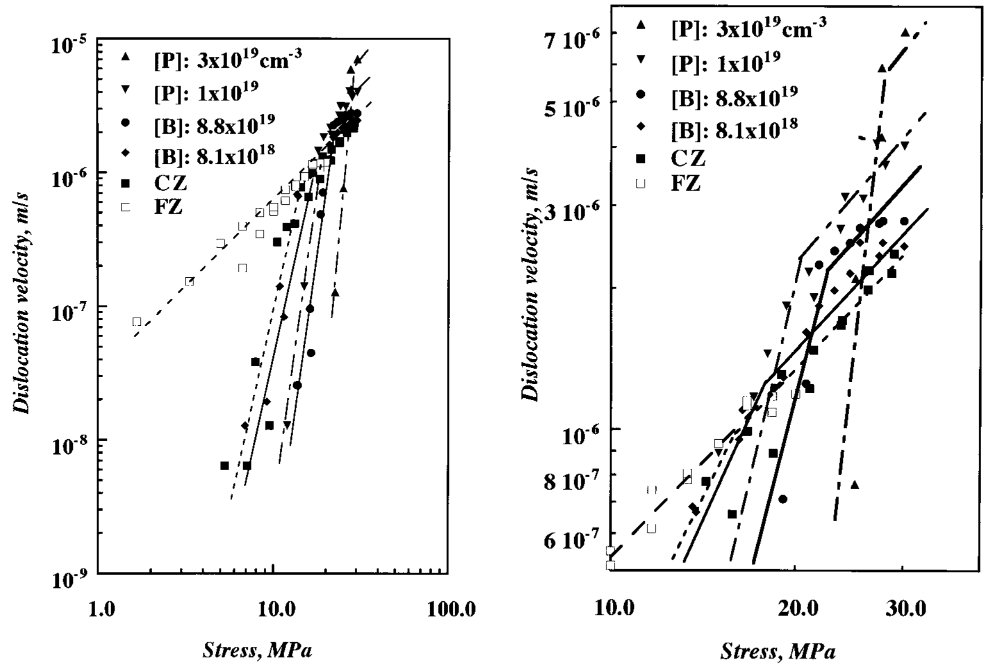


Figure 2. Variation in the critical stress at 800 °C for 60° dislocations against the concentrations of B and P impurities in Si crystals. The triangles and circles denote dislocations in B- and P-doped Si, respectively, and the solid and open symbols relate to CZ- and FZ-Si, respectively.

higher than $\approx 1 \times 10^{19}$ cm^{-3} effectively suppress dislocation generation. The critical stress for dislocation generation observed within B- and P-doped crystals with concentrations lower than 1×10^{19} cm^{-3} should originate mainly from the effect of oxygen (O) impurities, since the CZ-Si crystals contain O atoms with a concentration of about 10^{18} cm^{-3}. However, it is noted that B and P impurities themselves have a slight effect of suppressing dislocation generation for such low concentrations. The absence of dislocation generation from a scratch or surface flaw under low stress is observed also for dislocations in Si, GaAs, and InP doped with certain kinds of impurity, as reported previously [1, 3, 5, 6]. This has been interpreted in terms of the immobilization of dislocations due to locking by impurity atoms segregated along the dislocations [1, 5]. Possibly, some stable structure may be constructed in cooperation with a few impurities or intrinsic point defects, as calculated by Heggie *et al* for P impurity [7]. Here, the immobilization of dislocations by B and P impurities becomes remarkable when the concentration exceeds 1×10^{19} cm^{-3}, an order of magnitude higher than the O concentration, in spite of the large capacity for dislocation immobilization. This may be due to the rate of diffusion of B and P impurities being lower than that of O impurity.

The distance travelled by the leading dislocation in an array under a given stress divided by the stressing duration is taken to be the velocity of the dislocation under that stress. Figure 3 shows the velocities of 60° dislocations at 800 °C plotted against the resolved shear stress. For undoped FZ-Si the logarithm of the velocity is linear with respect to the logarithm of the stress for the whole range investigated. The dislocation velocity is described as a function of stress τ according to the empirical law $v \propto \tau^m$, where $m \approx 1$, which is same as the result previously reported [1]. The velocity of 60° dislocations in undoped CZ-Si, P-doped FZ-Si, and B-doped CZ-Si increases rapidly once the stress exceeds the critical stress for dislocation generation, and shows a break, depending on the impurity concentration. Such rapid increase in velocity with stress relates to the process of release of dislocations from the impurity-immobilized state. Beyond the break, the velocity increases rather slowly with increasing stress at a comparable rate to that for 60° dislocations in undoped FZ-Si. As seen in figure 3(b), in such a stress range where dislocation motion is free from the impurity immobilization effect, it is seen that the velocity of dislocations in P-doped crystals becomes faster, compared to those for undoped CZ-Si and FZ-Si, with increasing P concentration as previously reported [1, 3]. In addition, it is found that in B-doped crystals the velocity of dislocations also increases with increasing B



(a) (b)

Figure 3. (a) Velocities of 60° dislocations, in various Si crystals at 800 °C, as functions of the resolved shear stress. The travelling distance of the leading dislocation in an array under a given stress divided by the stressing duration was taken to be the dislocation velocity under that stress. (b) The velocity versus stress relation enlarged for the stress range 10–40 MPa.

concentration. It is well known that for semiconductors the dislocation velocity is influenced in a variety of ways by electrically active impurities through the formation and/or migration of kinks as an elementary process of dislocation motion. If the enhanced velocity of dislocations detected in B-doped Si is related to such a mechanism, then a donor level will be associated with a kink site in Si, in addition to the idea that a kink in P-doped Si has an acceptor level proposed by Hirsch [8] and Jones [9]. This may also be related to the reduction of kink formation energy through an elastic interaction with impurity atoms as discussed in connection with the solution softening in bcc metals and alloys [10].

To help a comprehensive understanding, the dynamic characteristics of dislocations in Si heavily doped with B and P impurities observed in the present work are shown qualitatively in table 1 together with those for the cases of O, nitrogen (N), and carbon (C) impurities previously reported [1]. As shown in the table, P and B impurities have remarkable effects on the dislocation immobilization when the concentration is higher than 10^{19} and 5×10^{19} cm^{-3}, respectively, in comparison with O and N impurities. P and B impurities enhance the dislocation velocity while O, C, and N have no effect.

4. Conclusions

The dynamic behaviour of dislocations in Si heavily doped with acceptor B and donor P impurities is investigated. Dislocation generation is strongly suppressed in Si when the B and P concentrations exceed 1×10^{19} cm^{-3}, which is interpreted in terms of dislocation locking due

Table 1. Qualitative comparison of the effects of various impurities on the dislocation immobilization and the velocity under high stress where the dislocation is free from the influence of immobilization by impurity. The table gives the impurity concentration at which the immobilization becomes effective.

Impurity	Immobilization	Velocity
O	Yes $>5 \times 10^{17}$ cm^{-3}	No effect
N	Yes $>10^{15}$ cm^{-3}	No effect
C	No	No effect
P	Stronger than that of O $>10^{19}$ cm^{-3}	Strong enhancement
B	Stronger than that of O $>5 \times 10^{19}$ cm^{-3}	Slight enhancement

to impurity segregation. The velocity of dislocations in B-doped Si increases with increasing concentration; these results are similar to those previously reported for Si highly doped with P impurity.

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