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Impurity effects on dislocation activities in Si

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Abstract

The dynamic activity of dislocations in Si doped with acceptor, donor and neutral impurities to various concentrations up to 2.5 × 10^{20} cm^{-3} is investigated by using the etch-pit technique, in comparison with that in undoped Si. Dislocation generation from a surface scratch is strongly suppressed when the concentration of B, P and As impurities exceeds 1 × 10^{19} cm^{-3}, which is interpreted in terms of dislocation locking due to impurity segregation. Dislocation velocity increases on increasing the concentration in B, P, As and Sb impurities.

1. Introduction

Establishing knowledge on dislocation–impurity interaction is important from both the fundamental and practical viewpoints for development of semiconductor technology. A well-known example, the dislocation–oxygen interaction in Si, has been well investigated in terms of the dislocation immobilization due to preferential segregation [1, 2] and the findings are widely used as basic knowledge in Si crystal growth and device fabrication processes. In current advanced Si technology, wafers prepared from large-diameter crystals heavily doped with electrical impurities are used as substrate material for the epitaxial growth of clean materials without grown-in defects. Conversely, easy generation of dislocations within large-diameter Si wafers is detrimental to the device fabrication process because of the self-weighting. Recently, dislocation-free Si crystals have been successfully grown without the Dash necking process (which was a standard procedure for over 40 years), by the Czochralski technique with heavy doping of certain impurities [3–5]. However, far less is known on the dynamic activities of dislocations in Si heavily doped with electrically active impurities.

The present author has recently reported preliminary results on the characteristic suppression of dislocation generation and the enhancement of dislocation velocities in Si crystals doped with some impurities, investigated by means of the etch-pit technique [6–8]. This paper reports on the impurity effects on the generation and velocity of dislocations in Si crystals doped with acceptor (B), donor (P, As and Sb) and neutral (Ge) impurities to various concentrations up to 2.5 × 10^{20} cm^{-3}, in comparison with those in undoped and O-doped Czochralski-grown (Cz) Si crystals.

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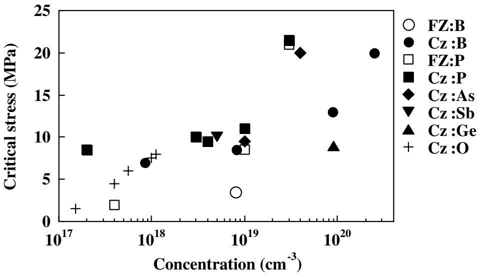

Figure 1. Variation in the critical stress for generation of 60° dislocations at 800 °C against the concentration of impurities B, P, As, Sb, Ge and O in Si crystals.

2. Experimental procedure

Specimens were prepared from dislocation-free Cz Si crystals doped with various concentrations of B, P, As, Sb and Ge. Specimens of float-zone-grown (FZ) Si doped with B and P impurities and undoped Cz Si were also investigated 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 drawn on the chemically polished (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 in order to introduce preferential nucleation centres for dislocations at stressing. The specimen was stressed at elevated temperature by means of three-point bending in a vacuum. The generation and motion of dislocations from the scratch were detected by observing the etch pits developed by modified Sirtl etchant [9] at 20 °C. The geometry of the specimens as well as the details of the experimental procedure are described in previous articles [6–8].

3. Dislocation generation

The generation of 60° dislocations from a scratch under various stresses was investigated. There exists a certain critical stress for the generation of dislocations in Cz Si and FZ Si with impurities; meanwhile no appreciable critical stress is measured for dislocation generation in undoped FZ Si.

Figure 1 shows the dependence of the critical stress for dislocation generation at 800 °C on the concentration of B, P, As, Sb and Ge impurities. Data for various concentrations of oxygen (O) impurity are also included in the figure. The critical stress increases with increasing O concentration and becomes 7–8 MPa at about 10^{18} cm^{-3}, the usual level of O concentration in Cz Si. The critical stress starts to increase remarkably when the B, P and As concentrations exceed 1×10^{19} cm^{-3}, which implies that B, P and As, with concentration higher than $\approx 1 \times 10^{19}$ cm^{-3}, effectively prohibit generation of dislocations. Thus, the critical stress for dislocation generation observed within crystals doped with B, P, As and Sb to less than 1×10^{19} cm^{-3} can be understood to originate mainly from the effect of O impurity. However, it is noted that B, P and probably As and Sb impurities themselves have a slight suppression effect on dislocation generation even in such a low concentration. In comparison with the case for such impurities, the critical stress for dislocations in Si doped with Ge is 7–8 MPa, the same as the critical stress for undoped Cz Si. This may mean that Ge impurity does not have as strong an effect of suppression of dislocation generation. Indeed, in the dilute alloys $Ge_{0.004}Si_{0.996}$, strong suppression of dislocation generation has not been observed [10]. The absence of dislocation generation from a scratch or surface flaw under low stress is observed

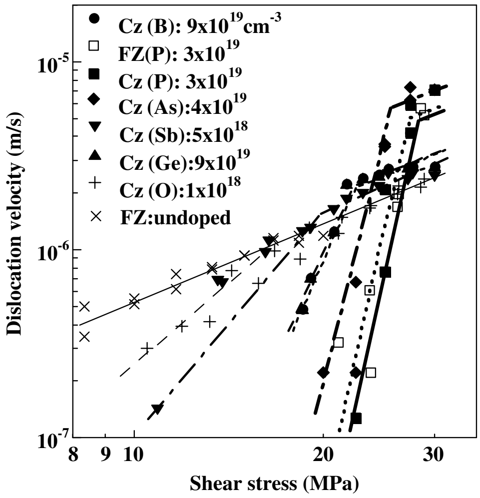

Figure 2. Velocities of 60° dislocations in various Si crystals at 800 °C as a function of the resolved shear stress.

also for dislocations in Si [1], GaAs [11] and InP [12] doped with certain kinds of impurity. Dislocations nucleated around the scratch are immobilized due to the segregation of impurity atoms along the dislocation lines while the crystal is being heated to the test temperature. The critical stress for generation can be understood as the stress for unlocking dislocations from such a state to allow them to penetrate into the matrix crystal [1, 11, 12]. Possibly some stable structure may be constructed in cooperation with a few impurities or intrinsic point defects, as predicted theoretically by Heggie *et al* [13]. Indeed, the analysis of the temperature dependence of the unlocking stress of aged dislocations indicates the existence of locking agents of interaction energy 3–4 eV with densities of around 1–3 $\times$ 10^5 cm^{-1} along a dislocation line in Si doped with certain impurities [7].

4. Dislocation velocity

Figure 2 shows the velocities of 60° dislocations at 800 °C in various Si crystals plotted against the resolved shear stress. The dislocation velocity v in undoped FZ Si 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 impurity-doped Si increases rapidly once the stress exceeds the critical stress value for dislocation generation and shows a break, which depends on the impurity species and concentration. Such rapid increase in the velocity with respect to the stress relates to the process of unlocking dislocations from the impurity-immobilized state. Beyond the break, the velocity increases rather slowly with increase in the stress at a comparable rate to that of 60° dislocations in undoped FZ Si. In such a stress range where dislocation motion is free from the impurity immobilization effect, as seen in figure 3, the velocity of dislocations in Si doped with P, As and Sb impurities increases with increase in the concentration as reported previously [1, 5, 7, 14–17]. Additionally, the dislocation velocity in B-doped Si increases gradually with increase in the B concentration [5–7]. However, in B- and P-doped Si of the highest concentration investigated, the dislocation velocity is influenced by the immobilization by the impurities. In Ge-doped Si, the dislocation velocity increases slightly.

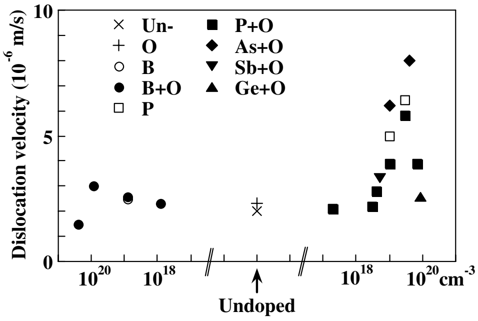

Figure 3. Velocities of 60° dislocations under a shear stress of 30 MPa at 800 °C in Si crystals: the dependence on the electrical type and concentration of the main impurities.

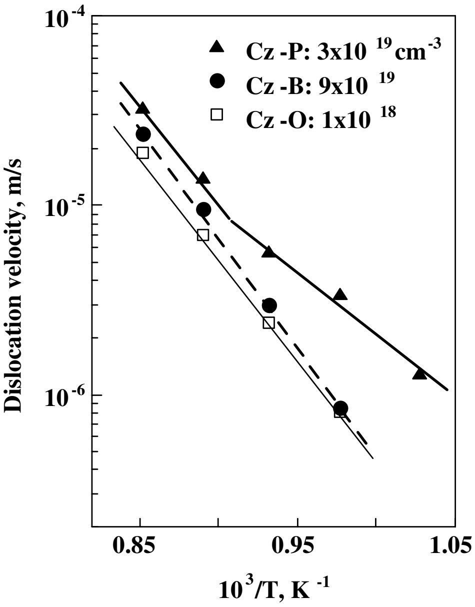

Figure 4. Velocities of 60° dislocations in B-doped, P-doped and undoped Cz Si under a shear stress of 30 MPa against the reciprocal temperature.

Figure 4 shows the velocities of 60° dislocations in Cz Si doped with B to 9×10^{19} cm^{-3} and P to 3×10^{19} cm^{-3} under a stress of 30 MPa plotted against the reciprocal temperature, together with the results for undoped Cz Si. It is seen that dislocations move far faster in P-doped Si than in B-doped and undoped Si at temperatures lower than about 800 °C. The velocity enhancement is attributed to the electrical effect of donor impurities through the formation and/or migration of kinks as an elementary process of dislocation motion. An acceptor level will be associated with a kink site in Si as proposed by Hirsch [18] and Jones [19]. In contrast, even at temperatures higher than 800 °C the dislocation velocities in B- and P-doped Si are larger than those of dislocations in undoped Si. Such enhancement of dislocation velocity observed in heavily impurity-doped Si may not be originating from the above mechanism, since a break of the temperature dependence of the dislocation velocity in P-doped Si is seen in figure 3. The kink configuration of a dislocation is probably concerned in heavily impurity-doped semiconductors; where the doping level is extremely high, the sample can be regarded as rather like a dilute solid solution.

5. Summary

The dynamic activity of dislocations in Si heavily doped with acceptor (B), donor (P, As, Sb) and neutral (Ge) impurities is investigated. Suppression of the dislocation generation from a surface scratch is found for Si doped with B, P and As with a concentration higher than 1×10^{19} cm^{-3}. The critical stress for dislocation generation increases with B, P and As concentration, which is interpreted in terms of dislocation immobilization due to impurity segregation. The velocity of dislocations in Si increases with increase in the concentration of not only the donor but also the acceptor impurities at elevated temperatures.

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