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Dislocation–impurity interaction in Si

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Abstract

Dynamic dislocation–impurity interactions in CZ–Si doped with light impurity (N), acceptor (B), donor (P, As, Sb) and neutral (Ge) impurities were investigated in comparison with those in undoped CZ–Si. Dislocation generation was effectively suppressed in B-, P- and As-doped Si when the concentration was higher than 10^{19} cm^{-3}, while Ge impurity did not strongly suppress dislocation generation. Dislocations were immobilized by the stable complexes formed through the impurity segregation and reaction. It was found that B and N impurities promptly form strong locking agents, while P and As impurities form highly dense locking agents along dislocations. Dislocation velocity in Si doped with electrically active impurities increased with increasing concentrations of not only the donor (P, As, Sb) but also the acceptor (B) impurities in the temperature range of 650–950 °C. N and Ge impurities had no or little effect on the velocity of dislocations in motion. Co-doping of Si with Ge and B was effective for suppression of dislocation generation and retardation of dislocation velocity at low temperatures.

Keywords: Dislocation–impurity interaction; Generation; Immobilization; Velocity; Impurity segregation; Si

1. Introduction

Understanding of dislocation–impurity interaction in crystals and wafers with large diameters is important for advanced silicon technology. This interaction has two aspects: (1) the effect of dislocations on the spatial distribution of impurities, as in gettering, defect reaction and complex formation, which is essential for dislocation-engineering; (2) the effect of impurities on the dynamic properties of dislocations, which is essential in the growth of dislocation-free crystals and the suppression of slippage and warpage during wafer processing. However, far less is known about the interaction of dislocations and impurities, except for those of oxygen impurity in Si crystals. The dislocation–oxygen interaction in Si is well known in terms of dislocation immobilization due to preferential segregation [1,2] and, indeed, basic knowledge of this is widely applied in the growth of bulk crystals and thin films and in device fabrication processing. The present author's group succeeded in growing dislocation-free Si crystals by the Czochralski (CZ) method without the conventional Dash-necking process with heavy doping of boron (B) impurity at a concentration higher than 10^{18} cm^{-3} [3] for the growth of heavy Si crystals with large diameter. The present author has previously reported the suppression of dislocation generation and the enhancement of dislocation velocities by certain kinds of impurities in Si [4–6]. The present paper details the dynamic interactions between dislocations and impurities in CZ–Si doped with light impurity (N) and acceptor (B), donor (P, As, Sb) and neutral (Ge) impurities at various concentrations up to 2.5×10^{20} cm^{-3}, as well as those in CZ–Si co-doped with Ge and B, hereafter termed (Ge + B) co-doped.

2. Experimental

Specimens were prepared from dislocation-free CZ–Si crystals doped with various concentrations of B, P, As, Sb, N and Ge and co-doped with Ge and B at concentrations of 4×10^{19} and 9×10^{18} cm^{-3}, respectively. All the CZ–Si crystals contained oxygen (O) impurity at a concentration of $\approx 1 \times 10^{18}$ cm^{-3}. High purity float-zone-grown (FZ)-Si and undoped CZ–Si were also employed for purposes of comparison. Specimens were sectioned into rectangular shapes 2 mm × 3 mm × 15 mm with the long axis in the $[1\bar{1}0]$ direction and the side surfaces parallel to the (1 1 1) and $(1 1 \bar{2})$ planes. Scratches were drawn on the chemically polished $(1 1 1)/(\bar{1}\bar{1}\bar{1})$ surfaces in the $[1\bar{1}0]$ direction at room temperature with a diamond stylus to introduce preferential dislocation nucleation sites. The specimen was stressed at an elevated temperature by means of three-point bending in a vacuum. The motion of dislocations from the scratch was investigated by observing etch pits detected by a modified

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Sirtl etchant [7]. Details of the experimental procedures and the crystal growth have been described in previous reports [3–5].

3. Results and discussion

3.1. Critical stress for dislocation generation

A certain critical stress exists for generation of dislocations from a scratch in CZ–Si doped with certain impurities. No appreciable critical stress, however, has been measured for dislocation generation in high purity FZ–Si. Fig. 1 shows the dependence of the critical stress for dislocation generation at 900 °C on the concentration of doped impurities in CZ–Si crystals. Data for various concentrations of oxygen (O) impurity are also included in the figure. The critical stress increases with increasing O concentration and becomes 8 MPa at about 10^{18} cm^{-3}, the standard level of O concentration in CZ–Si. The critical stress starts to increase remarkably when B, P and As concentrations exceed 1×10^{19} cm^{-3}. This means that B, P and As impurities at concentrations higher than $\approx 1 \times 10^{19}$ cm^{-3} effectively suppress the generation of dislocations. Thus, the critical stress for dislocation generation observed within crystals doped with concentrations of B, P and As impurities less than 1×10^{19} cm^{-3} can be understood to be mainly due to the effect of O impurity. B and P impurities in FZ–Si have also been found to suppress dislocation generation [6]. However, the critical stresses for dislocation generation in FZ–Si are lower than those in CZ–Si. The suppression of dislocation generation by Sb impurity is not clear because its solubility limit into Si is lower than those of B, P and As impurities.

In Ge-doped Si, the magnitude of the critical stress for dislocation generation is 8 MPa, i.e., the same as the critical stress for undoped CZ–Si, and increases slightly to $\approx$10 MPa when the Ge concentration exceeds 10^{20} cm^{-3}. However, Ge impurity even at a high concentration of 2.5×10^{20} cm^{-3} is not effective for suppression of dislocation generation. Indeed, in the dilute SiGe alloys with Ge content of 0.004, strong suppression of dislocation generation has not been observed [8]. Contrarily, in (Ge + B) co-doped CZ–Si, the critical stress of dislocation generation is higher than that in Si independently doped with either B or Ge. This shows the effect of (Ge + B) co-doping effect on the suppression of dislocation generation, though such effect is weaker than that observed at 800 °C [5].

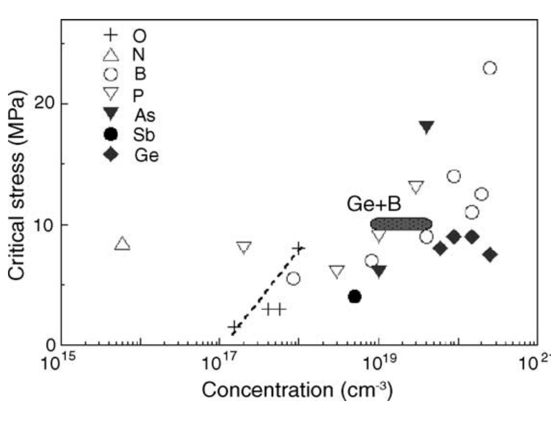

Fig. 1. Variation in the critical stress for generation of 60° dislocations at 900 °C against the concentration of N, B, P, As, Sb, Ge and O impurities in CZ–Si crystals. The ellipse denotes the critical stress in Ge and B co-doped Si at concentrations of 4×10^{19} and 9×10^{18} cm^{-3}, respectively.

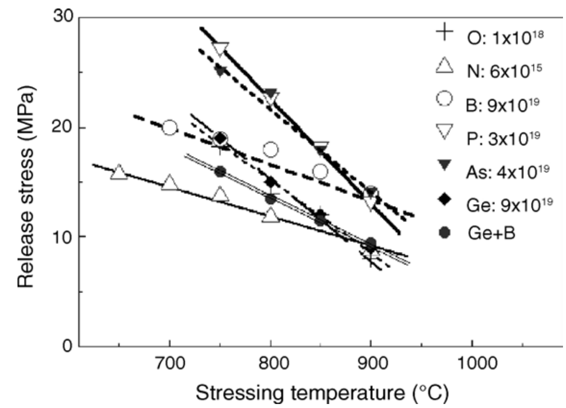

Fig. 2. Stressing temperature dependence of release stress τ_R for dislocations aged at 900 °C for 15 min in various types of CZ–Si. (Ge + B) denotes the results for CZ–Si co-doped with Ge and B at concentrations of 4×10^{19} and 9×10^{18} cm^{-3}, respectively.

In N-doped CZ–Si, the critical stress for dislocation generation is 9 MPa, comparable to or somewhat higher than that in undoped CZ–Si.

3.2. Dislocation immobilization

The absence of dislocation generation from a scratch or surface flaw under low stress has been observed for dislocations in several semiconductors doped with certain kinds of impurity (see review [1]). Dislocations are nucleated around a scratch/surface flaw and immobilized due to the impurity segregation along the dislocations even while the crystal is being heated to the test temperature [1,5,6]. The observed critical stress for dislocation generation should be understood as the stress required to release a dislocation from the immobilized state and to penetrate into the matrix crystal, which can be detected macroscopically as dislocation generation from the scratch. This stress is termed release stress τ_R. The characteristic features of dislocation–impurity interaction can be evaluated through the analysis of the stressing temperature dependence of the release stress of aged dislocations.

Fig. 2 shows the release stress against the stressing temperature for dislocations in various Si crystals aged at 900 °C for 15 min. The release stress decreases linearly with an increase in the stressing temperature, showing that the process is thermally activated. A theory of the thermally activated release of dislocations from locking agents gives the following relation between the release stress τ_R and the temperature T:

$$\tau_R = \frac{[E - k_B T \ln(LN\nu/\Gamma)]N}{b^2}, \quad (1)$$

where E is the maximum interaction energy between a dislocation and a locking agent, L the length of the dislocation, N the mean density of locking agents along the dislocation line,