The effect of dopants on the brittle-to-ductile transition in silicon single crystals

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Abstract. The brittle-to-ductile transition (BDT) in boron, antimony and arsenic doped Cz silicon crystals has been experimentally studied, respectively. The BDT temperatures in antimony and arsenic doped silicon wafers are lower than that in a non-doped wafer while the BDT temperature in a boron doped wafer is almost the same as that in the non-doped wafer. The activation energy was obtained from the strain rate dependence of the BDT temperature. It was found that the values of the activation energy in the antimony and arsenic doped wafers are lower than that in the non-doped and boron doped wafers, indicating that the dislocation velocity in the antimony and arsenic doped silicon is faster than that in the non-doped while the dislocation velocity in the boron doped is the same as that in the non-doped. The effect of increasing in dislocation velocity on the BDT temperature was calculated by two-dimensional discrete dislocation dynamics simulations, indicating that the increasing in dislocation velocity decreases the BDT temperature in silicon single crystals.

1. Introduction

Silicon crystals have been used as model crystals to understand the mechanism behind the brittle-to-ductile transition (BDT) behaviour since St. John [1] demonstrated that they show a very sharp BDT. Many studies after his work revealed that the controlling process of the BDT is dislocation glide, deducing from the fact that the values of the activation energy obtained were close to those for dislocation glide [2-4]. Roberts et al [5] showed that the BDT temperature in phosphorous doped silicon was lower than that in the non-doped one and the activation energy obtained from the strain rate dependence of the BDT temperature was close to that for dislocation glide. It implied that the BDT behaviour was affected by doped elements via change of dislocation velocity. Since several kinds of dopants are added in silicon crystals for commercial use, it is necessary to investigate the
effect of dopants on the BDT behaviour. In this study, the effect of p-type dopant (boron) and n-type dopants (arsenic or antimony) on the BDT behaviour will be discussed based on the dislocation shielding theory [6]. The effect of the change in dislocation velocity on the BDT was also investigated by two-dimensional discrete dislocation dynamics simulations.

2. Experimental Procedure

Specimens were prepared from one-side mirror polished (001) wafers grown by Czochralski technique without dopants \( \left( 1 \times 10^{15} \text{atoms/cm}^3 \right) \) of boron remained and those with dopants of boron \( \left( 3.6 \times 10^{19} \text{atoms/cm}^3 \right) \), antimony \( \left( 2.2 \times 10^{18} \text{atoms/cm}^3 \right) \) and arsenic \( \left( 2.8 \times 10^{18} \text{atoms/cm}^3 \right) \). Rectangular specimens of \( 8 \times 35 \times 0.62 \text{mm}^3 \) were cut out from the wafers for subsequent three-point bending tests. Fracture tests were carried out at temperatures between 770K and 1120K. The cross-head speed (CHS) was set to be 0.002mm/min, 0.02mm/min and 0.2mm/min, respectively. Apparent fracture toughness was obtained by following equations.

\[
K_\text{Q} = \sigma_f \sqrt{2 \pi a f(\xi)}, \quad \text{with} \quad \xi = \frac{a}{w} \quad \text{and} \quad f(\xi) = 1.090 - 1.735 \xi^2 + 8.20 \xi^3 - 14.18 \xi^4 - 14.57 \xi^4, \quad (1)
\]

where \( \sigma_f \) is the fracture stress, \( a \) is the notch depth and \( w \) is the specimen height. The BDT temperature was determined as one at which the highest value of apparent fracture toughness in each CHS was achieved. The activation energy for the controlling process of the BDT was obtained from Arrhenius plots of the logarithm of the CHS against the inverse temperature.

3. Results and Discussions

Figures 1 (a)-(d) show temperature dependence of the apparent fracture toughness in boron doped, non-doped, antimony doped and arsenic doped silicon single crystals respectively. The apparent fracture toughness increases with increasing temperature, from the lowest valued of 1.3MPa.m^{1/2}. The BDT temperature, \( T_{\text{BDT}} \), is defined as the highest apparent fracture toughness, in this study. The relationship between the BDT temperatures in each specimen was found to be: \( T_{\text{BDT, As}} \leq T_{\text{BDT, Sb}} \leq T_{\text{BDT, B}} = T_{\text{BDT, non}} \) at any strain rate. It was thus found that p-type dopant (boron) does not affect the BDT temperature while n-type dopants (arsenic and antimony) decrease the BDT temperature. The same kind of result that n-type dopants show lower BDT temperature was obtained by Roberts et al although the dopant is not the same as those employed in the present study but phosphorous [5]. In order to investigate the influence of doping on the rate determining process, i.e., dislocation mobility, the activation energy was measured from the deformation rate (CHS) dependence of the BDT temperature obtained in this study.
Figure 2 shows Arrhenius plots of the logarithms of the CHS against the inverse BDT temperature. The slopes of each Arrhenius plot indicate the activation energy of 1.6eV, 2.0eV, and 2.3eV for arsenic doped, antimony doped and boron/non-doped silicon crystals, respectively. The relationship between the activation energy, $E$, in each specimen is: $E_{\text{As}} < E_{\text{Sb}} < E_{\text{B}} = E_{\text{non}}$. The tendency of the activation energy is the same as that of the BDT temperature. The results indicate that the activation energy for dislocation glide is decreased by the antimony and arsenic doping but not changed by the boron doping. In order to investigate the effect of the decrease in the activation energy for dislocation glide on the BDT temperature, the temperature dependence of fracture toughness was calculated by two-dimensional discrete dislocation dynamic simulations. The detail of the simulation is shown elsewhere [7,8].

Figure 3 shows the temperature dependence of the fracture toughness calculated by using the two-dimensional model. The symbols of triangle, square and circle demonstrate results from the activation energy of 1.6eV, 2.0eV, and 2.3eV for dislocation glide, respectively, corresponding to that for arsenic, antimony and boron/non-doped silicon crystals. It is to be noted here that the BDT temperature decreased with decreasing in the activation energy for dislocation glide.
Therefore, it is concluded that the decrease in the BDT temperature in n-type doped silicon is due to the increase in the dislocation velocity in silicon single crystals.

4. Conclusions
The effect of dopants on the BDT behaviour in silicon crystals was investigated. The BDT temperature decreased with n-type dopants. The activation energy obtained from the rate dependence of the BDT temperature indicates that the dislocation velocity in n-type (antimony or arsenic doped) silicon are faster than that in non-doped silicon. Two-dimensional discrete dislocation dynamics simulations indicate that increasing in dislocation velocity decreases the BDT temperature. It is concluded that the decrease in the BDT temperature in n-type silicon is due to the increase in the dislocation velocity.

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