Impurity locking of dislocations in silicon

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Oxygen in Czochralski silicon (Cz-Si) can retard or suppress dislocation motion and hence can improve the mechanical stability of the material [1]. Furthermore, the intentional addition of nitrogen to silicon is of considerable interest since it is believed that it can control vacancy concentration, affect oxygen precipitation and improve mechanical strength. In this work, locking of dislocations by oxygen in Cz-Si and by nitrogen in float-zone silicon (FZ-Si) has been investigated over a wide range of annealing times and temperatures.

Locking experiments on Cz-Si with three different oxygen concentrations (2.6, 6.3 and 10.4 x 10^{17} cm⁻³) were performed at temperatures from 350 to 850°C. The unlocking stress was found to display five distinct regimes. From the temperature dependence of the saturation unlocking stress, the binding enthalpy of the oxygen species to the dislocation has been deduced. Two values of binding enthalpy have been found and these correspond to the high temperature (650 to 850°C) and the low temperature (350 to 550°C) regime respectively.

Experimental results indicate that at temperatures below approximately 650°C enhanced oxygen transport to dislocations takes place. Numerical simulations indicate that the effective diffusivity is different from "normal" diffusivity and can be several orders of magnitude larger (Figure 1). At lower temperatures the effective diffusivity becomes dependent on the oxygen concentration and has an activation energy of approximately 1.5 eV.

Dislocation locking experiments were performed on N-doped FZ-Si with a nitrogen concentration of 2.2×10^{15} cm⁻³ annealed at temperatures between 550 and 830°C. It has been found that the locking effect due to the nitrogen is similar in magnitude to that of oxygen in Cz-Si, even though the nitrogen concentration is two orders of magnitude lower.

The stress applied to unlock the dislocations was found to increase approximately linearly with annealing time, with a rate that has a strong temperature dependence. The unlocking stress saturates to a value of approximately 50MPa for all temperatures investigated. Interestingly, this is in contrast to the locking due to oxygen in Cz-Si, in which the saturation stress depends on temperature. In particular, Figure 2 shows that for temperatures greater than approximately 750°C, nitrogen is capable of locking the dislocations more efficiently than oxygen, despite the lower nitrogen concentration. This property of nitrogen could be of considerable importance for FZ-Si technology, as one of the disadvantages of using FZ-grown silicon in microelectronics is notably the weak resistance of FZ wafers against warpage, especially if compared with Cz-grown materials.

From an Arrhenius plot of the initial rise in stress with time against temperature (Figure 3), the activation energy for nitrogen transport to the dislocations has been found. An expression for the diffusivity of a possible diffusing species has been deduced. The value of the activation energy measured in this work is much lower than values in the literature [3]. The results will be discussed in terms of the nature of the species responsible for diffusion in the temperature ranges considered.



Figure 1: Diffusivity of oxygen in silicon as a function of reciprocal temperature. The closed points are the values found in this work. The three different data sets were obtained using specimens of different oxygen concentration. The open points are from the literature [2].



Figure 2: Comparison of dislocation locking between oxygen in Cz-Si and nitrogen in FZ-Si.



Figure 3: An Arrhenius plot of the increase in unlocking stress as a function of time against temperature for N-doped FZ-Si [4].

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