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Diffusion and Precipitation of Oxygen Atoms in Heavily Impurity doped Silicon Crystals

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1. Introduction

Interstitial oxygen atoms incorporated into Czochralski-grown silicon (Cz-Si) crystals become supersaturated and tend to precipitate during crystal growth and also the fabrication of semiconductor devices. Oxygen precipitation phenomena have extensively been investigated since oxygen precipitates have a crucial role for internal gettering of undesirable impurities. It has been well recognized that oxygen precipitation is enhanced by heavy doping of *p*-type impurity, boron (B), while that is suppressed by heavy doping of *n*-type impurities such as antimony (Sb), arsenic (As) and phosphorus (P). However, the mechanism of oxygen precipitation in the heavily doped Si is unclear. The purposes of this study are to clarify the influences of dopants on diffusion and precipitate nucleation of oxygen atoms in heavily doped Cz-Si.

2. Diffusion of oxygen in heavily doped Si

Influences of B, As and Sb on oxygen diffusivity at 500−800°C, at which the nucleation process in the oxygen precipitation becomes dominant, were investigated in heavily doped Cz-Si wafers with concentration of $10^{18}-10^{19}$ atoms/cm^3. In the experiment, the out-diffusion profile of oxygen was measured by secondary ion mass spectrometry after prolonged heat treatments, and then the oxygen diffusivity was determined from analysis of the profile using the Fick's second law. The obtained results are as follows.

2.1. Effect of heavy B doping on oxygen diffusion

The oxygen diffusivity shows a non-monotonic temperature dependence below 800°C by heavy B doping, i.e., a minimum appears at around 600−700°C. In this temperature range, nucleation of oxide precipitates was found to be effectively enhanced by heavy B doping. It is thus concluded that retardation of oxygen diffusion in heavily B-doped specimen is due to enhanced formation of immobile oxygen aggregates.

2.2. Effect of heavy As and Sb doping on oxygen diffusion

The oxygen diffusivity was reduced by the heavy As and Sb doping, being larger reduction at lower temperatures. Hence the apparent activation energy of oxygen diffusion below 800°C is larger than that at higher temperatures depending on dopant species. On the assumption that the dopants act as trap sites for oxygen atoms, binding energy of oxygen to each dopant and effective trap-site density were obtained from analysis of the increase of activation energy. The obtained binding energies of oxygen to As and Sb are 0.6 and 1.3 eV, respectively. On the other hand, effective trap-site density in heavily Sb-doped specimen was lower than that in the heavily As-doped specimen. This is interpreted to be related with strain effect of dopants.

3. Precipitate nucleation of oxygen in heavily doped Si

The nucleation of oxide precipitates in Cz-Si wafers heavily doped with B, As, and Sb at 600 − 700°C has been investigated. The nucleus density was determined by measuring precipitate density after growth due to two-step heat-treatment at 800°C and 1000°C. The dependence of the nucleation on the annealing time at 600 − 700°C was analyzed with the use of chemical rate equations in order to obtain the density and the size of critical nuclei and rate constants for nucleation reaction.

3.1. Effect of heavy B doping on precipitate nucleation

The B doping effect on critical nucleus density at 700°C appears at the concentrations higher than about 3×10^{18} atoms/cm^3 where the density of nucleus is proportional to the square of B concentration. This demonstrates that the heavy B doping introduces heterogeneous nucleus containing two B atoms. Besides, the heavy B doping increased rate constant for nucleation reaction due to large capture radius of the heterogeneous nucleus for diffused oxygen atoms. It was thus found that enhancement of oxygen precipitation by heavy B doping is caused by the heterogeneous nucleation.

3.2. Effect of heavy As and Sb doping on precipitate nucleation

The density and the size of critical nuclei in heavily As- and Sb-doped wafers were similar to that of lightly B-doped wafer at 600 − 700°C, and hence As and Sb had no effect on the nuclei. The lower the nucleation temperature, the higher the density of critical nuclei and the smaller the nucleus size. On the other hand, the rate constants for nucleation were diminished by the heavy doping, and correlated with the dopant-retarded oxygen diffusion. It was thus found that suppression of oxygen precipitation by heavy As and Sb doping is caused by the retardation of oxygen diffusion.

In conclusion, influences of dopants on diffusion and precipitation of oxygen atoms in heavily doped Cz-Si were quantitatively clarified in this study. From the point of view of industrial technology, the obtained results are useful for control of oxygen precipitation in heavily doped substrates of Si epitaxial wafers.