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Segregation of Ge in B and Ge codoped Czochralski-Si crystal growth

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[Introduction] It was found that doping of Ge in Si is beneficial as it improves the mechanical strength, minority carrier lifetime and enhances the quality of Si by reacting with point defects [1]. All the above-mentioned beneficial effects are varied as a function of Ge concentration in Si [1]. To control the Ge concentration in Si crystal, one should have a clear understanding about segregation of Ge in Si crystal growth. But, unfortunately the segregation of Ge in Si is completely mystery as the effective segregation coefficient (k_{eff}) of Ge in Si is rarely reported and the value is widely scattered from 0.33 to 0.72. In the present investigation, we investigated the k_{eff} of Ge in heavily Ge codoped CZ-Si crystal growth. The experimental data were comparatively analyzed with theoretically calculated equilibrium segregation coefficient (k_o).

[Experiment] B and Ge codoped <100> Si crystals with various initial Ge concentrations, C_l^{Ge}, ((3×10^{19} to 3×10^{21} cm^{-3}) and fixed initial B concentration (1.3×10^{16} cm^{-3}) in Si melt were grown by CZ method. The pulling rates were decreased for the heavily Ge codoped CZ-Si to avoid cellular growth. The ingots were sliced as wafers and chemically mirror finished using acid mixture of HF and HNO_3 (1:5). The Ge concentrations of the wafers were measured by Field Emission Electron Probe Microanalysis (FE-EPMA) using JEOL JXA-8530F system.

The k_{eff} of Ge was calculated by fitting the FE-EPMA data in the normal freezing equation, $C_s^{Ge}=C_l^{Ge}k_{eff}(1-g)^{(keff-1)}$, where g is the solidified fraction and C_s^{Ge} is the Ge concentration in the crystal. For the fitting, the C_l^{Ge} should be precisely estimated as it is quite difficult due to Ge evaporation at high temperature and this uncertainty causes large errors in the estimated k_{eff}. To avoid this uncertainty, the k_{eff} of Ge was calculated by taking logarithmic ratio of Ge concentration between top and bottom part of the crystal without using the estimated C_l^{Ge} values [2]. The k_o of Ge was calculated using Thurmond and Struther's partitioning equations [3]. The k_{eff} of Ge was calculated as a function of growth rates using BPS theory and compared with experimental data.

[Results and discussion] Fig. 1 shows the Ge distribution in a heavily Ge codoped CZ-Si grown from Si melt with C_l^{Ge} of 3×10^{19} cm^{-3}. The estimated values of k_{eff} by the two methods are almost in the same range and it shows that the estimated C_l^{Ge} was accurate. For the following discussion, the k_{eff} values estimated by normal freezing equation were considered. The estimated k_{eff} of Ge was 0.21 for the crystal with C_l^{Ge} of 3×10^{19} cm^{-3} and relatively increased up to 0.46 when the C_l^{Ge} increased up to 1.52×10^{21} cm^{-3}. For the crystal with very high C_l^{Ge} of 3×10^{21} cm^{-3}, the k_{eff} of Ge decreased to 0.28, however,the fitting was not good with the R value of 0.95 when compared to other crystals. This is due to the fact that the pulling rate was frequently varied intentionally in the range of 0.08 to 0.15 mm/min to control the diameter of the crystal. The calculated k_o value of Ge was 0.2 and k_{eff} for the crystal with C_l^{Ge} of 3×10^{19} cm^{-3} was almost in the same range. But, the estimated k_{eff} for the crystals with C_l^{Ge} higher than 3×10^{19} cm^{-3} was quite larger than the calculated k_o value. Ge-Ge pair formation is considered as a possible reason for the higher k_{eff} in the heavily Ge codoped CZ-Si. The variation of k_{eff} with growth rates was calculated using BPS theory and it followed the same tendency of experimentally observed variations of k_{eff} for the heavily Ge codoped crystal growth.

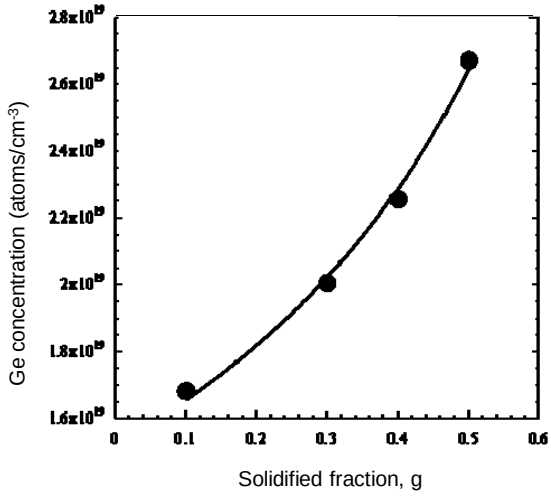

Fig.1 Ge concentration in a Si crystal grown from Si melt with initial Ge concentration of 3×10^{19} atoms/cm^{-3}.

References
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