Evaluation of the point defect bulk recombination rate by ion implantation at high temperatures

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During ion implantation of boron with 120keV, Frenkel pairs are generated with a rate of approx. 137 Frenkel pairs per implanted boron atom. When the implantation is done at diffusion temperatures, the generated silicon self-interstitials and vacancies can recombine. At the same time, they can migrate into the bulk and to the surface of the wafer where they will be consumed. The remaining point defects serve as diffusion vehicles and thus cause an enhancement of the diffusion of boron by several orders of magnitude /1/. This implantation enhancement is similar to that observed during RTA but allows detailed studies because of the much larger effects.

Detailed studies based on a dynamic pair diffusion model have shown that the remaining point defects reach an equilibrium condition in a time negligible to the overall process time. This equilibrium can be described by the equations

$$\mathrm{div}\, D_I C_I^{eq}\, \mathrm{grad}\, s_I = K_B \cdot C_I^{eq} \cdot C_V^{eq} \cdot (s_I s_V - 1) - G_I$$

$$\mathrm{div}\, D_V C_V^{eq}\, \mathrm{grad}\, s_V = K_B \cdot C_I^{eq} \cdot C_V^{eq} \cdot (s_I s_V - 1) - G_V$$

where the symbols D, C^{eq}, s, and G denote diffusion coefficients, equilibrium concentrations, point defect oversaturations, and generation terms due to the ion implantation. The indices I and V stand for silicon self-interstitials and vacancies, respectively. The oversaturation of silicon self-interstitials and vacancies is assumed to be one at the surfaces of the wafer. In these equations, the product of the point defect diffusion coefficients times their equilibrium concentrations are very well known. For the product of the bulk recombination rate K_B times the equilibrium concentrations, however, no reliable value was available up to now.

As a main result of this analysis, we could determine reliable values for this product in the range from 800°C to 900°C by comparing numerical solutions of the equations given above to measurements. In Fig.1, the measured profile of an implantation at 900°C with an energy of 120keV, a dose of 10^{15}cm^{-2} during 1h is shown together with the respective simulation and an implantation profile obtained at room temperature. The peak value of the oversaturation of silicon self-interstitials is 1200 for this example.

The excellent agreement obtained supports the basic assumptions of pair diffusion. Measurements at 800 and 850°C suggested a value for the product of the bulk reaction rate times the point defect equilibrium concentrations of $K_B \cdot C_I^{eq} \cdot C_V^{eq} \sim 7.1 \cdot 10^{44} \cdot \exp(-8.95eV/kT)\ cm^{-3}s^{-1}$ (Fig.2). The 90% confidence interval for the activation energy is 7.44eV < EA < 8.95eV due to the small numbers of experiments performed up to now. If we assume that the activation energies of the equilibrium concentrations are on the order of 4.4eV for silicon self-interstitials and 2eV for vacancies, the activation energy of the bulk reaction rate must be on the order of 3.55eV. This value is significantly higher than the value of 1.4eV reported by Antoniadis and Moskowitz /2/.

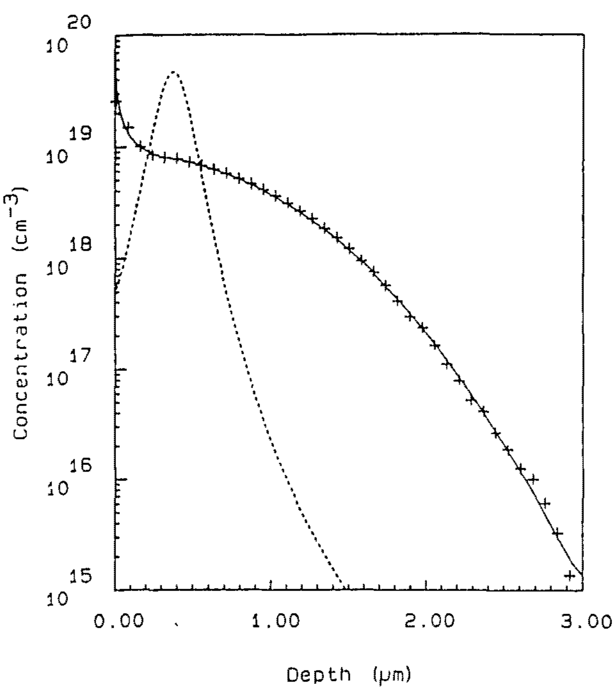

Fig.1: Simulation of ion implantation with $10^{15}cm^{-2}$ at 900°C for 1h (——) together with measurements (+) and the room temperature implantation profile (-----)

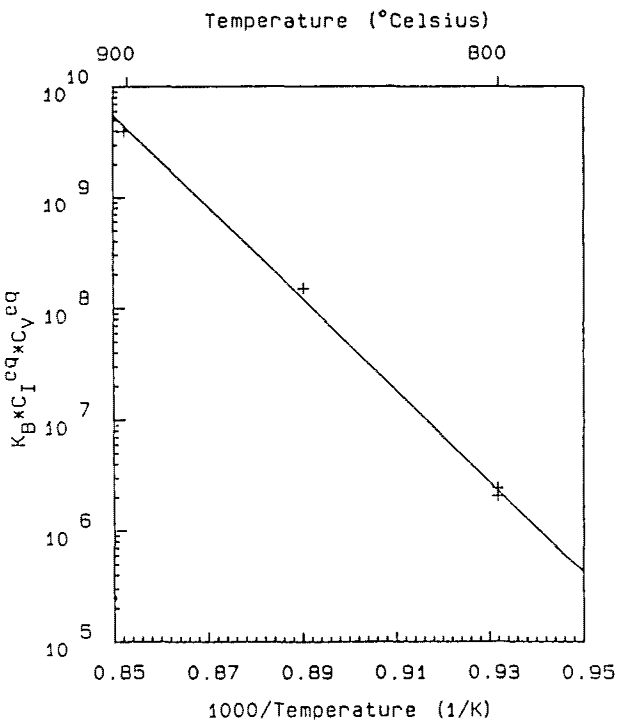

Fig.2: Product of the point defect bulk recombination rate times the equilibrium concentrations of interstitials and vacancies as a function of temperature

/1/ R. Schork, P. Pichler, A. Kluge, H. Ryssel, 'Radiation-Enhanced Diffusion During High-Temperature Ion Implantation', accepted for publication in Nuclear Instruments and Methods in Physics Research, Section B, Beam Interactions with Materials and Atoms.

/2/ D.A. Antoniadis, I. Moskowitz, 'Diffusion of substitutional impurities in silicon at short oxidation times: An insight into point defect kinetics', J.Appl.Phys. v.53, no.10, pp.6788-6796 (1982)