ROLE OF INTRINSIC POINT DEFECTS IN CREATION OF DEEP LEVEL DEFECTS

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The last experimental data allows to suppose that the intrinsic point defects (IPD) play an essential role in creation of deep level defects (DLD) during heat treatment of silicon. Their low concentration does not allow to determine their origin by electron microscopy, electron paramagnetic resonance and other traditional methods. The aim of this paper is to investigate the effect of IPD supersaturation of silicon on DLD creation during heat treatment.

We have investigated the defects formed during heat treatment of p—n structures and dislocation-free float-zone silicon single crystals of n-type conductivity. To obtain IPD supersaturation the crystals and structures were annealed at 850—1250° C for 0.5—40 h in a chlorine-containing atmosphere. Detailed conditions of the treatments were given in /1/.

The defects' parameters were studied by capacitance spectroscopy and diffuse gamma-ray scattering (0.003 nm wavelength) /2/. The asymmetric diffuse tails have been observed in the silicon surface regions of 0.2—1.2 mm in thickness during a measurement of the rocking curves. The appearance of the tails is connected with diffuse gamma-ray scattering on the displacement field resulted from the defects formed by IPDs. The creation of vacancy defects increases the diffuse-scattering intensity at angles smaller than the ideal Bragg angle ($\Theta - \Theta_B < 0$) and the creation of self-intersititial defects increases the latter at angles larger than Θ_B ($\Theta - \Theta_B > 0$). Thus diffuse gamma-ray scattering allows to investigate a change of the IPD supersaturation degree of silicon.

DLD parameters were investigated in the samples characterized by asymmetric diffuse tails. The Schottky-barrier or p—n structures were used for such measurements. Fig. 1 shows DLTS-spectra of the samples supersaturated by defects of the vacancy (A) and interstitial (B) type. The activation energy (E) and the electron capture cross section (σ) were calculated from the temperature dependencies of the thermal emission rates of electrons from deep levels: E1=0.535 eV and $\sigma 1 = 1.6 \cdot 10^{-15}$ cm^2, E4=0.277 eV and $\sigma 4 = 1.9 \cdot 10^{-17}$ cm^2, E7=0.192 eV and $\sigma 7 = 1.1 \cdot 10^{-15}$ cm^2. Three of the same DLDs were formed in both groups of the samples but different heat treatment changed their concentration: M1=M4=$(0.5—1.6) \cdot 10^{11}$ cm^{-3} and M7=$(0.6—1.7) \cdot 10^{12}$ cm^{-3} in group A, M1=M4=$(0.9—4.3) \cdot 10^{11}$ cm^{-3} and M7=$(1.4—5.2) \cdot 10^{10}$ cm^{-3} in group B. The diffuse gamma-ray scattering and the capacitance spectroscopy data comparison shows that the E1 and E4 defects creation is due to the supersaturation of silicon by self-interstitials and the E7 defect creation by vacansies.

The effect of the change of diffuse gamma-ray intensity from the range of smaller angles to the larger ones has been observed in the surface layers of the neutron irradiated and heat treated samples. The reflectivity distribution along the axis of the crystal growth is shown in fig. 2 for the deviation of 15″ relative to the ideal Bragg angle (R_-, R_+). The observed dependencies are explained by

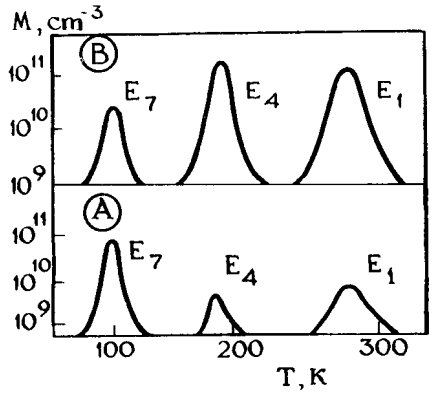

Fig. 1

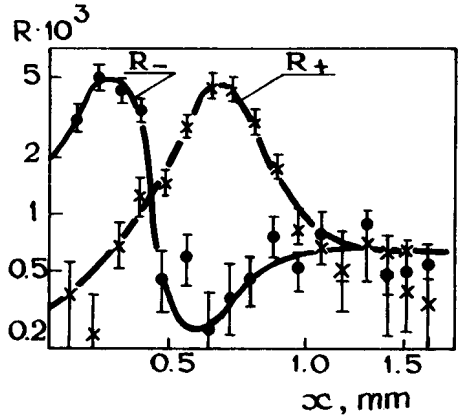

Fig. 2

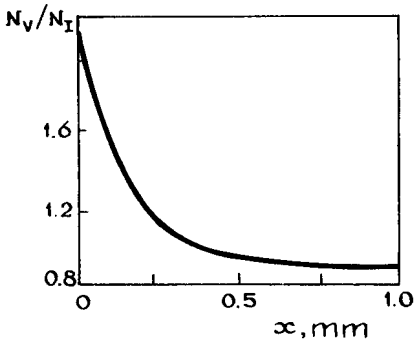

Fig. 3

the change of the type of dominant IPDs responsible for the defects creation in the studied layers. Defects of the vacancy type are dominant in the surface layers of 0.4 mm in thickness. Interstitial defects are dominant in layers from 0.5 to 1.1 mm.

Let us consider the model of the creation of IPD-associated defects. To obtain the IPD concentration distribution during heat treatment, one has to solve simultaneously the following continuity equations for vacancies and interstitials:

$$\frac{\partial V}{\partial t} = D_V \frac{\partial^2 V}{\partial x^2} - k_{bi}(IV - I^* V^*), \tag{1}$$

$$\frac{\partial I}{\partial t} = D_i \frac{\partial^2 I}{\partial x^2} - k_{bi}(IV - I^* V^*), \tag{2}$$

and has to choose appropriate initial $I/I^*(t=0)=3$, $V/V^*(t=0)=1.2$, and boundary conditions $I/I^*(x=0)=6.6\cdot10^{-9}\exp(2.52/kT)t^{-1/4}+1$, $V/V^*(x=0)=3.14t^{-0.176}+1$, where k — Boltzmann constant, I and V — interstitial and vacancy concentrations, I^* and V^* — their values at thermal equilibrium, D_i and D_V — their diffusivity, k_{bi} — the bimolecular generation-recombination rate, $t_{bi}=1/k_{bi}V^*=7.2\cdot10^4$ s— interstitial bulk lifetime, $I^*/V^*=0.1$, $D_i/D_V=10$, $D_i=2\cdot10^{-7}$ cm²/s. During the cooling of the sample one can consider that the IPD distribution is changed only due to the creation of the vacancy and interstitial defects. In the first approximation the defects' sizes do not depend on IPD supersaturation and their concentration is characterized by linear dependence and $k_i=k_V=$const, $N_i=k_i(I-I^*)$, $N_V=k_V(V-V^*)$. Fig. 3 shows the solution of the task. There is a good correspondence between the data of fig. 2 and fig. 3.

Diffuse gamma-ray scattering and capacitance spectroscopy data comparison allows to determine the origin of DLDs induced during the heat treatment of silicon and to maintain that the excessive lattice defects play the main role during DLD creation. To confirm this conslusion, a model of DLD creation, due to supersaturation of silicon by IPDs, has been proposed.

REFERENCES

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2. *Kurbakov A. I. et al.* Sov. Tech. Phys. Lett., 1988. V. 14. 1929.