

## AMORPHIZATION AND STRESS KINETICS IN ION IMPLANTED CRYSTALLINE SOLIDS

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**Abstract.** Nowadays, ion implantation is widely used for doping and modification of semiconductors. Ion bombardment induced amorphization, strain and stress of semiconductors is the subject of many articles dealing with ion implantation. Dependence of the stress (or strain) on the ion dose, energy, kind of ions, stress relaxation processes are the key problems that are solved in the recent articles on this subject. Usually stress in the crystalline silicon increases with the dose of ion irradiation and maximum values of stress ( $10^8 - 10^9$  Pa) are reached in the region of the dose close to the amorphization dose. After initial growth of the stress in ion implanted region further irradiation induces relaxation of the stress and maximum of the stress-dose can be found for many ion combinations. If the mass of ions increases the maximum usually is shifted to the lower dose region. Stresses in the plane for thin samples depend on the biaxial strain. On the other hand, strain in the perpendicular direction to the plane is measured experimentally. Poisson relation is used to express strain in plane using the values of strain in the perpendicular direction. It should be mentioned as well that plastic flow of the material can contribute to the strain in plane if the crystal is saturated by radiation defects. As the result, some errors in the determination of the real values of strain can be induced. To avoid these uncertainties analytical expression directly for the stress in plane can be constructed. Strain in plane in the present paper expressed using elementary volume related to the point defect and stress-strain dependence is defined taking in account relaxation processes in the ion irradiated solid.

**Keywords:** stress, ion implantation, radiation defects.

### Introduction

We have investigated the ion beam induced amorphization process in solid during bombardment with light, medium and heavy mass ions. Ions accelerated to energy in the keV or MeV range, deposit a considerable amount of their energy into elastic collisions to target atoms during this process. This deposition results in the formation of point defects (Frenkel pairs) and cluster of them in the crystalline matrix during ion irradiation. The accumulation of defects into a crystalline solid can lead to the formation of an amorphous phase. The kinetics of formation of the amorphous phase may be described by a classical mechanism of nucleation and growth [1-2]. The nucleation has been ascribed to the prompt part of the collision cascade while the growth of the amorphous layer has been ascribed to long living defects.

Studies with Rutherford backscattering confirm that two stages of the formation of defects can be depicted. The first stage appears when flux  $\Phi \leq \Phi_C$  ( $\Phi_C$  is critical flux), Frenkel pairs concentration  $C$  changes monotonously. In the second stage ( $\Phi \geq \Phi_C$ ) the concentration of defects gradually increased [3-4]. This indicates that the defect production in the predamaged crystal is more efficient than in a virgin crystal, suggesting that the newly produced defects can destabilize the crystal and cause the formation of disordered zones of increased size. Such a process produces about eight times more displacements than can be directly generated by nuclear collisions. This process of amorphization can be related with the collapsing [4-5] of crystal zones: these zones, being between disorderly oriented clusters, are compressed and their lattice is deformed [3; 6-8]. Lattice compression [9-10] is explained by interface crystal – amorphous movement and thermal spikes [7-8].

### Materials and Methods

Guided by our observation of accelerated growth of damage, we have modeled the damage built up phenomenologically by assuming that the production rate of stable defects is proportional to the concentration  $C$  of the existing defects:

$$\frac{dC}{d\Phi} = F_n n_o^{-1} (1 - C) + \alpha j^{-1} C - \beta n_o j^{-1} C^2, \quad (1)$$

where  $F_n$  – the number of defects, created by irradiation in one unit layer;  
 $n_o$  – the particle density in the crystal,

$j$  – ion flux;  
 $\alpha, \beta$  – phenomenological parameters.

The first component describes the rate of generation in the cascades of elastic collisions, the second component describes the collapsing of crystal zones, and the third one describes the recombination of vacancies and interstitials.

The solution of Eq. (1) may be obtained from the following conditions:

$$C(\Phi \rightarrow 0) = 0, \quad C(\Phi \rightarrow \infty) = 1 \quad (2)$$

and

$$\left. \frac{dC}{d\Phi} \right|_{\Phi \rightarrow \infty} = 0. \quad (3)$$

The following equality results from the equation (3):

$$\alpha = \beta n_0. \quad (4)$$

From equation (1-4) Frenkel pair concentration can be expressed as

$$C = \frac{1 - e^{-\frac{(1+C_0)\Phi}{\Phi_0}}}{1 + C_0^{-1} e^{-\frac{(1+C_0)\Phi}{\Phi_0}}}. \quad (5)$$

where  $C_0 \equiv F_n j (\alpha n_0)^{-1}$  and  $\Phi \equiv j \alpha^{-1}$ .

## Results and Discussion

**Stress in ion implanted crystals.** We assume that the point defects are the sources of strain in the ion implanted surface layer. Elastic forces emerge near the point defect – vacancies induce compression and interstitial tension in the crystal lattice. Let us note relative increment of the atomic volume due to vacancy as  $\Delta\Omega_v\Omega^{-1}$ , due to interstitial as  $\Delta\Omega_i\Omega^{-1}$  and implanted ion as  $\Delta\Omega_{ion}\Omega^{-1}$  ( $\Omega$  is the atomic volume in the crystal). Usually  $|\Delta\Omega_v| < \Delta\Omega_i$ . Ion irradiation induces local expansion of the lattice. It should be noted as well that expansion of the lattice depends on the concentration (5) of Frenkel pairs and implanted ions  $C_{ion}$ . Taking in account all component biaxial intrinsic strain tensor in the plain ( $\varepsilon_{11}^* = \varepsilon_{22}^* \equiv \varepsilon_{in}^*$ ) we can express as following:

$$\varepsilon_{in}^* = \frac{1}{3} \left( C \frac{\Delta\Omega_F}{\Omega} + C_{ion} \frac{\Delta\Omega_{ion}}{\Omega} \right), \quad (6)$$

where  $\Delta\Omega_F\Omega^{-1} = \Delta\Omega_i\Omega^{-1} - |\Delta\Omega_v|\Omega^{-1}$ .

Ion concentration can be defined from

$$C_{ion} = F_{ion}(x_3) n_h^{-1} \phi, \quad (7)$$

where  $n_h$  – interstitial hole density

$F_{ion}(x_3)$  – is the function describing ion distribution versus depth  $x_3$ .

Expression for the planar stress ( $\delta_{11} = \delta_{22} = \delta_{in}$ ) relaxation can be found from the Boltzmann – Volterra's integral equation:

$$\delta_{in} = -\frac{Y}{1-\nu} \left( \varepsilon_{in}^*(\Phi) - \int_0^\phi \Gamma(\Phi - \Phi') \varepsilon_{in}^*(\Phi') d\Phi' \right), \quad (8)$$

where  $Y$  – Young's modulus of integral transformation of (8).

Let us assume that elastic viscous medium can be described using a model Maxwell. Nucleus of transformation in this case can be expressed as an exponential function

$$\Gamma(\Phi) = \Phi_r^{-1} \exp(-\Phi/\Phi_r), \quad (9)$$

where  $\Phi_r = 6(1-\nu)j\eta/Y$  – characteristic flux of relaxation, where  $\eta$  is the viscosity of the material.

Integral stress in the ion implanted layer of thickness  $d$  is:  $S = \int_0^d \sigma_{in}(x_3) dx_3$ .

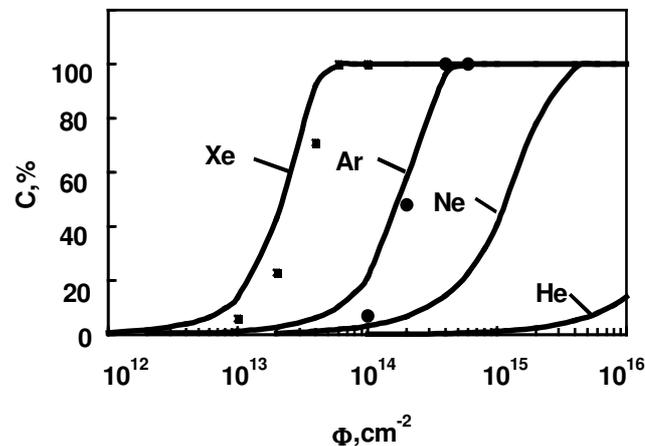


Fig. 1. Calculated defect concentration dependence in silicon on the flux of ion irradiation: the experimental values are marked by symbols ■, ●, ◆, Δ (ion energy 570 keV (Xe) and 250 keV (Ar), ion flux  $\leq 0.5 \mu\text{Acm}^{-2}$ ).

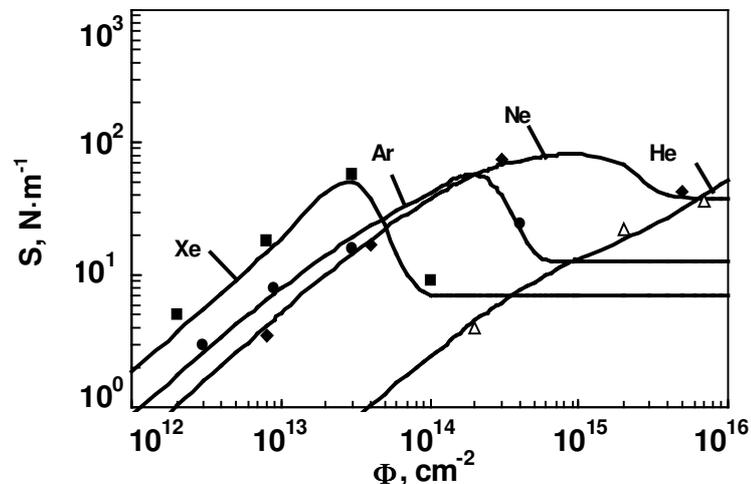


Fig. 2. Calculated integral stress dependence in silicon: the experimental values are marked by symbols ■, ●, ◆, Δ [9; 11] (ion energy 220 keV, ion flux  $1 \mu\text{Acm}^{-2}$ ).

## Conclusions

The transformation of silicon to the amorphous state by implanted ions into Si (100) at room temperature was studied theoretically. The critical role of point defects (Frenkel pair) produced by ion implantation in enhanced diffusion also have been recognized. A theoretical model of production and relaxation of stress in ion – implanted silicon is proposed. The integrated stress acting in a damaged layer has been studied as the function of the Xe ions.

## References

1. EerNisse E. P., Sensitive technique for studying ion-implantation damage, *Applied Physics Letters*, Vol 18, No.12, 1971, pp. 581-583.
2. Пранявичюс Л., Дудонис Ю. “Модификация свойств твердых тел ионными пучками”, Вильнюс, Мокслас, 1980, 242 с. (In Russian).
3. Tamulevičius S., Požėla I., Jankauskas J., Integral stress in ion-implanted silicon. *Applied Physics*, Vol 31, No.7, 1998, pp. 2991-2996.
4. Болтакс Б.И. “Диффузия и точечные дефекты в полупроводниках”, Ленинград, Наука, 1972 581с. (In Russian).
5. Harlmeier F., Bolse W. Ion beam induced amorphization in  $\alpha$  quartz, *Applied Physics* Vol 83, No.7, 1998, pp. 4049-4054.
6. Chason E., Picraux S. T., et. al. Ion beams in silicon processing and characterization, *J. Applied Physics*, Vol. 81, No. 10, 1997, pp. 6513-6561.
7. Domkus V., L. Pranevičius L. *Mechaniškeskie napriazhenie v implantirovanix tverdex telax*, (Vilnius, Mokslas, - 1990, 155 p. (In Russian).
8. Girdauskienė D., Požėla I. *Lietuvos mokslas ir pramonė, Konferencijos pranešimų medžiaga* (Kaunas, KTU, 1998), pp. 330-332. (In Lithuanian)
9. Гирдаускене Д., Пожела И. *Lietuvos fizikos žurnalas*, T.39, No.1, 1999, pp. 69-73. (In Russian).
10. Girdauskienė D., Požėla I. *Defektų susidarymas Si jonais švitinamame silicyje, Spinduliuotės ir medžiagos sąveika, Resp. konf. Pranešimų medžiaga* (Kaunas, KTU, 1999), pp. 109-111. (In Lithuanian)
11. Bai G., Nicolet M.-A. Defects production and annealing in self – implanted Si, *Applied Physics*., Vol 70, No. 2, 1991, pp. 649-655.