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Physics

Inelastic Properties of Monocrystalline Si-Ge Alloys

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ABSTRACT. Internal friction and shear modulus temperature and amplitude dependences of monocrystalline Si-Ge alloys have been investigated. It was established that monocrystalline silicon doped with Ge caused decrease of the activation characteristics of the internal friction relaxation processes. Increase of Ge concentration in Si-structure also caused a decrease of the values of critical amplitudes of oscillatory deformation. The causes of decrease of the structure defects migration energy in monocrystalline Si-Ge alloys were analysed. © *2007 Bull. Georg. Natl. Acad. Sci.*

Key words: *silicon, germanium, internal friction, shear modulus, dislocation.*

Dislocation and point defects-vacancy and impurity atoms interaction significantly determine the physical properties of Si-Ge system monoctrystals in which formation and transformation of structure defects are controlled by covalent forces. Different aspects of the mechanism of structural defects formation, interaction and thermal activation of various structural defects were revealed during the investigation of properties of monoctrystalline Si [1-3]. In the present study we have investigated the temperature and amplitude dependence of internal friction (IF) and shear modulus of monoctrystalline Si+1at%Ge and Si+2at%Ge specimens. Measurements of the logarithmic decrement of damping and frequency of torsional oscillations were carried out with laboratory equipment. Measurements were performed in the range of torsional oscillations 0.5-5 Hz frequency and the temperature interval 300-1000 K. The research objects are Si-Ge monoctrystals obtained by the Czochralski method and characterized by *p*-type conductivity, hole concentration $\sim 10^{15}$ cm^{-3} and dislocation density $\sim 10^{4}$ cm^{-2}.

The temperature dependence of IF at the 0.8 Hz frequency of crystalline Si is characterized by maxima at temperatures of 380, 590, 710, 820, 940 and 1010 K (Fig. 1, curve 1). Temperatures of maxima change with the frequency change. The activation parameters of IF maxima are shown in Table 1. Significant decrease of IF maxima intensity is observed after annealing the samples in vacuum at 1000 K for 1 h. The cyclic deformation of monocrystalline Si specimens (number of cycles – 200, amplitude of oscilllation $\sim 5\times10^{-4}$) at 700 K sharply raises the intensity and width of IF maxima revealed in the vicinity of 710, 820, 940 and 1010 K temperatures.

Internal stress has a significant influence on diffusion activity of point defects, and activation parameters of migration of various dislocations observed during investigation of temperature and amplitude dependences of IF and shear modulus in monoctrystalline specimens of silicon. Internal friction maxima are revealed in monoctrystalline Si+1%at.Ge at temperatures 400, 550, 690, 880, 920 and 1010 K (Fig. 1, curve 2).

Annealing in vacuum at 1000K for 0.5h fully suppreses maximum in the nearness of 400 K and other maxima significantly decreases. The real structure of Si+1 at %. Ge alloy changes substantially due to the cycle deformation in the nearness of 670 K (amplitude of oscillation $\sim 1\times10^{-4}$, number of cycles - 100) expressed by a significant increase of the intensity of IF relaxation maxima in the range of 500-1100 K.

In Si+2at%Ge alloy IF spectrum maxima are observed in the low temperature range. Table 1 shows that with the

Table 1

Activation characteristics of IF maxima of monocrystalline Si-Ge alloys

Specimen	Temperature T_{max}, K	Activation energy, eV	Frequency factor, sec^{-1}
Si p-type monoctrystal [111]	380	0.90	$5 \cdot 10^{12}$
	590	1.40	$5.5 \cdot 10^{12}$
	710	1.70	$7 \cdot 10^{12}$
	820	1.85	$1.4 \cdot 10^{12}$
	940	2.10	$1 \cdot 10^{12}$
	1010	2.40	$9 \cdot 10^{12}$
Si+1at.%Ge p-type monoctrystal	400	0.90	$1 \cdot 10^{12}$
	550	1.40	$4 \cdot 10^{12}$
	690	1.65	$7 \cdot 10^{12}$
	880	1.80	$1.2 \cdot 10^{11}$
	920	2.05	$1 \cdot 10^{12}$
	1000	2.30	$2.3 \cdot 10^{12}$
Si+2at.%Ge p-type monoctrystal	380	0.85	$1 \cdot 10^{12}$
	570	1.40	$1 \cdot 10^{13}$
	685	1.60	$3.5 \cdot 10^{12}$
	770	1.70	$8 \cdot 10^{11}$
	845	1.95	$2.5 \cdot 10^{12}$
	950	2.20	$2.8 \cdot 10^{12}$

increase of Ge concentration in the lattice of Si activation energy and frequency factor of IF maxima decrease. After annealing at 1000 K in vacuum $\cong 10^{-3}$ Pa for 0.5 h IF maxima observed in the range of 400-570 K dissapear. Intensity of other maxima and high temperature background of IF decrease. Cycle deformation in the nearness of 670 K (number of cycles 100, at amplitude of oscillation 5×10^{-4}) raises the intensity of IF background and of maxima in the range of 500-1000 K.

In deformed specimens all IF maxima broaden caused by the creation of new centres of relaxation with close values of activation energy. Ge practically does not influence the carrier concentration and type of electric conductivity. The influence of Ge is observed in the formation of an internal stress field localized near Ge atoms. They cause the slowing process of phase transformation in the oxygen complexes and nucleation of oxygen donors in a wide temperature range [4, 5]. These conditions influence the origin of impurity atmospheres around dislocations and respectively on the activation characteristics of relaxation maxima and values of shear modulus of monocrystalline Si-Ge alloys. The noticed peculiarities are determined by germanium content and by main characteristics of temperature and by amplitude dependences of IF in undoped crystals of Si-Ge system alloys.

Amplitude dependence of IF and shear modulus have been investigated at the room temperature of Si-Ge alloys. On the curve of IF amplitude dependence of Si two intervals are observed: slight rise and sharp rise divided by a critical amplitude of torsion deformation, $\varepsilon_c \sim 8 \times 10^{-4}$ (Fig. 2, curve 1). At this amplitude the relative shear modulus decreases sharply and IF sigificantly increases. Starting from this amplitude, IF measured in the conditions of amplitude decrease of oscillatory deformation has hysteresis character, revealed as a difference of IF values measured at increasing and decreasing the values of amplitudes of oscillatory deformation. This difference increases under the

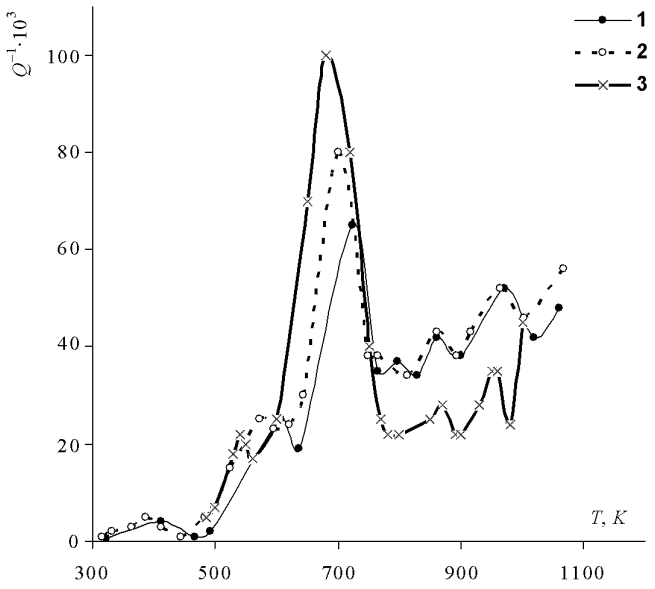

Fig. 1. Temperature dependence of internal friction of monoctrystalline Si-Ge alloys:
1 – Si, f = 1 Hz; 2 – Si+1at.%Ge, f = 1.2 Hz; 3 – Si+2at.%Ge, f = 0.8 Hz.

influence of high-amplitude cyclic deformation ~5×10^{-3} at 1000 K.

Suppression of the IF hysteresis is available by annealing of the samples for 1.5 h at 1273 K. Recovery of the IF hysteresis is realized after cyclic deformation at the amplitudes of oscillatory deformations of an order of $\varepsilon_c'' \sim 8\times10^{-3}$, at room temperature.

The main distinctive feature of amplitude dependence on the IF (Fig. 2, curve 2) and of Si samples alloyed with Ge consists in low values of critical amplitudes of oscillatory deformation. The IF hysteresis is better expressed in the alloyed Si.

Activation energy of IF maxima at 360 K is close to the migration energy of bivacancy in Si lattice [5]. Therefore it might be concluded that in the nearness of 360 K relaxation process is caused by motion of bivacancy in an external periodical stress field. It is supposed that in the nearness of 450 K energy scattering of oscillation is caused by the motion of the metastable complex of residual impurities and vacancies in the periodical mechanical field. There is a good coincidence between activation energy of IF maximum (450 K) and migration energy of complex vacancy-oxygen (~ 1.3 eV) [5].

The experiments have shown that in monocrystalline Si at the temperatures 710, 820, 940 and 1010 K relaxation maxima intensities depend on the amplitude of oscillation. Annealing at 1100 K for 0.5 h causes the reduction of IF maxima intensity. In the range 300-1100 K IF maxima are totally restored by cyclic deformation. They possess all properties of dislocation origin relaxation maxima observed in crystalline Si at the temperature range 700-1100 K, at 1 Hz frequency [3].

By the presence of different energies of creation and migration of single and double kinks at 60° and screw dislocations in Si may be supposed, which in Si-Ge crystals maxima at 710 and 820 K are caused by movement of geometrical kinks at 60° and screw dislocations. Maxima at 940 K and 1010 K may be explained by the creation and migration of double kinks at screw and 60° dislocations in an external stress field.

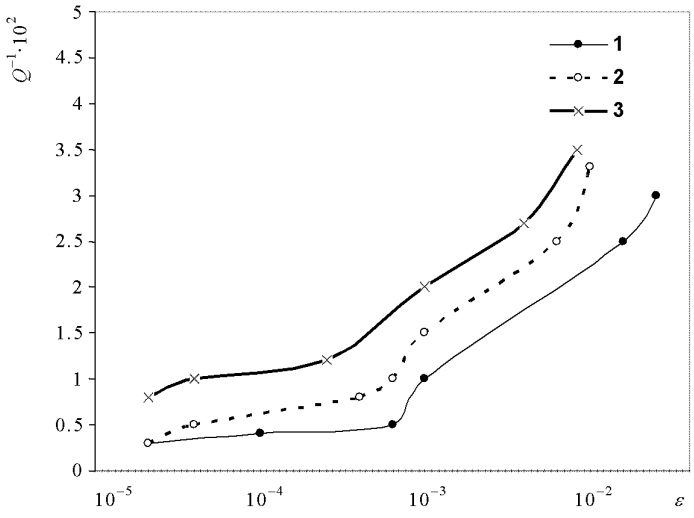

Fig. 2. Amplitude dependence of internal friction of monoctrystalline Si-Ge alloys:
1 – Si; 2 – Si+1at.%Ge; 3 – Si+2at.%Ge.

The experiments show that Ge in Si lattice causes reduction of effective activation energy and frequency factor IF maxima. The experiment results show that with the increase of amplitude of oscillations the height of the IF maxima increases and moves to low temperatures.

Thus, the investigation carried out in this study allows us to get information about the mechanism of scattering of mechanical oscillations connected with various types of dislocations, to determine the activation characteristics at 60° and screw. The experimental results are very important for understanding the physical processes caused by formation and transformation of dislocation structures and their interaction with various point defects. The results may be used for the prediction and control of charateristics of materials and devices on the basis of Si-Ge alloys.

ფიზიკა

მონოკრისტალური Si-Ge შენადნობების არადრეკადი თვისებები

ი. ყურაშვილი*, გ. ბოკუჩავა*, თ. მხეიძე*, ი. ბარათაშვილი, გ. დარსაველიძე***

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ნაშრომში შესწავლილია მონოკრისტალური Si-Ge შენადნობების შინაგანი ხახუნის და ძვრის მოდულის ტემპერატურული და ამპლიტუდური დამოკიდებულებები. დადგენილია, რომ გერმანიუმით ლეგირება იწვევს მონოკრისტალური სილიციუმის რელაქსაციური პროცესების აქტივაციური მახასიათებლების შემცირებას. გერმანიუმის კონცენტრაციის გაზრდით მცირდება რხევითი დეფორმაციის ამპლიტუდის კრიტიკული სიდიდეები. გაანალიზებულია Si-Ge შენადნობების სტრუქტურაში დეფექტების მიგრაციის ენერგიის შემცირების მიზეზები.

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