საქართველოს მეცნიერებათა ეროვნული აკადემიის მოამბე, 175, №2, 2007
BULLETIN OF THE GEORGIAN NATIONAL ACADEMY OF SCIENCES, 175, №2, 2007

Physics

Physico-Mechanical Properties of $Si_{0.85}Ge_{0.15}$:GaP Alloy

Guram Bokuchava*, Ia Kurashvili*, Ekaterine Sanaia*, Giorgi Darsavelidze*

* *F. Tavadze Institute of Metallurgy and Materials Science*

(Presented by Academy Member I. Baratashvili)

ABSTRACT. Internal friction and shear modulus temperature and amplitude dependences of $Si_{0.85}Ge_{0.15}$:GaP alloy were investigated. Relaxation processes of dislocation origin were revealed and their activation characteristics determined. The mechanism of internal friction relaxation processes was analyzed from the point of view of geometrical and double-kink migration on the screw and 60^0 dislocations. *© 2007 Bull. Georg. Natl. Acad. Sci.*

Key words: *doped silicon, internal friction, shear modulus, relaxation, activation energy, dislocation.*

Silicon-germanium alloys form a fully miscible solid solution with diamond crystal structure. These alloys have caused considerable interest due to their potential for band-gap and lattice-parameter engineering. Bulk SiGe alloys can be used as X-ray neutron monochromators and solar cells. They can also provide a lattice-matched substrate for SiGe epitaxial growth instead of Si.

It is known that doping of Si-Ge alloys by GaP [1] changes their thermoelectrical properties so that carrier concentration mobility in relation to thermal conductivity increases. According to this, it is possible to regulate the thermoelectrical properties of Si-Ge alloys in a wide range. Si-Ge solid solutions have been doped by GaP to obtain *n*-type crystals. The crystals are characterized by relatively low thermal conductivity and high Seebeck coefficient. It is remarkable that GaP-doped Si-Ge alloys are characterized by high-temperature diffusion activity of constituent components and high concentration and mobility of defects [2]. This determines various electrophysical parameters of the mentioned alloys. Therefore, it is necessary to carry out an investigation of the structural sensitivity of the physical properties in the initial state and after thermal treatment.

In this work we have studied the internal friction and relative shear modulus of GaP-doped Si-Ge alloy in the area of frequency of torsion oscillations of ~1Hz and at temperature range of 20-800°C. The measurements were carried out at the amplitude of oscillatory deformation $5 \cdot 10^{-5}$, at which internal friction intensity dependence on the amplitude of oscillation is not expected. The temperature spectrum of internal friction is rich in maxima. They are revealed at the temperatures of 100, 375, 390, 470, 560 and 670°C (Fig.1). The first maximum is characteristic of a silicon single crystal with perfect structure [3]. The relaxation internal friction of similar origin is revealed in Si-Ge system alloys with small concentration of germanium ($0 \le Ge \le 0.01$) [4]. The internal friction background at room temperature is characterized by a strong dependence on amplitude. This fact confirms its dislocation origin. The temperatures of revealed maxima in the spectrum of internal friction depend on oscillation frequency. So, they are of relaxation nature. The values of activation energy are determined by the method of frequency shift of relaxation internal friction maxima: 0.80; 1.40; 1.50; 1.65; 1.85; and 2.00eV. Their frequency factors are respectively: $5 \cdot 10^{11}$, $5 \cdot 10^{13}$, $2 \cdot 10^{12}$, $1 \cdot 10^{12}$ and $3 \cdot 10^{11} sec^{-1}$.

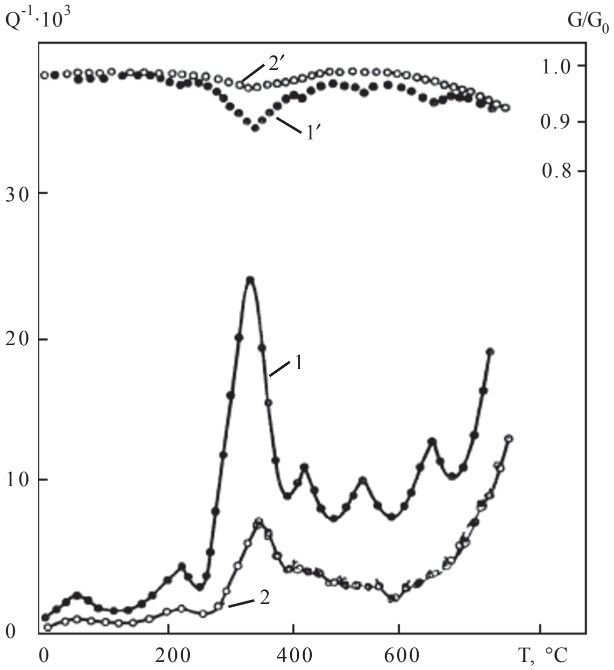

Fig. 1. Temperature spectra of internal friction (Q^{-1}) and relative shear modulus (G/G_0) of $Si_{0.85}Ge_{0.15}$:GaP alloy:
1.1′ – (Q^{-1}) and (G/G_0), initial state
2.2′ – (Q^{-1}) and (G/G_0), after annealing at 850°C, 50 hrs.

At the comparative high frequency (~5Hz) of oscillation in the temperature range of 300-700°C the internal friction background intensity decreases by ~15%. In the case of repeated measurements the critical values of oscillation amplitude increase, at which a significant increase of internal friction intensity begins.

During torsion oscillations, the deformation at room temperature practically has no effect on the shape and intensity of the internal friction spectrum obtained by repeated measurements. High temperature (~700^{0}C) cyclic deformation at the amplitude ~10^{-3} significantly increases the intensity of internal friction (~20%) and gives rise to broadening of the above-mentioned relaxation origin maxima. This variation is caused by microplastic deformation under a high amplitude of oscillation at the temperature 700°C. At high amplitude of oscillatory deformation generation of fresh dislocation is possible. Also, at high-amplitude oscillatory deformation the existing pinned dislocation segments may be detached from the pinning centers.

Annealing of alloys at 850°C for 50 hrs will cause the elimination of some relaxation centers, strong pinning of dislocations by point defects and their complexes. After long-term annealing, the intensity of internal friction maxima is significantly decreased. At temperature ~380°C there exists a low intensity maximum, but simultaneously the high-temperature internal friction background exponentially increases. After annealing a wide maximum is revealed at the temperature 380°C, which is characterized by the activation energy ~1.60eV, its frequency factor equalling ~$5 \cdot 10^{12}$sec^{-1}.

In the initial state a temperature spectrum of shear modulus with complex form was observed. Shear modulus decreases at temperatures of internal friction maxima. The local character of shear modulus decrease is due to a relaxation process taking place under the effect of temperature and periodical stress. Above 500°C steps and saturated areas exist on the shear modulus curve. Such changes of shear modulus are possible due to the high diffusion activities of oxygen, carbon and phosphorus atoms at high temperatures.

Table 1

The physico-mechanical characteristics of the GaP-doped Si-Ge alloy at fixed temperature

Si-Ge system alloy	Temperature, ^{0}C	Shear modulus, x10^3, kG/mm^2	I critical amplitude x10^4	II critical amplitude x10^4	Elasticity limit, kG/mm^2	
					I	II
$Si_{0.85}Ge_{0.15}$ doped with GaP	20	3.6	0.8	30	30.8	108
	150	3.45	0.6	25	21.7	86
	250	3.40	0.45	20	15.8	72
	350	3.30	0.4	13.0	13.2	43
	450	3.20	0.30	11.0	9.6	35
	550	3.15	0.20	10.0	6.3	31.5
	650	3.0	0.15	8.0	4.5	24

After annealing at 750°C for 50hrs there occurs dynamic strengthening of the $Si_{0.85}Ge_{0.15}$:GaP alloy. It is known [5] that in the process of high temperature annealing, migration of impurity atoms in the direction of dislocation cores accelerates. As a result, atmospheres of impurity atoms originate around the dislocations. In consequence of the above-mentioned dislocation blocking takes place. Owing to this, an increase of dynamical shear modulus is observed. Some physico-mechanical characteristics of the investigated sample are presented in Table 1.

Dislocation density increase of GaP doped Si-Ge alloy is achieved by deformation at high temperatures. This fact and the local, inhomogeneously distributed strains, generated by doping atoms have a strong effect on the distribution of technology impurities, and doping atoms and on the activation characteristics of the motion of dislocations. At 700°C high-amplitude deformation (~$5 \cdot 10^{-3}$), in conditions of 1.5Hrz frequency and 200 cycles of torsional oscillations of the $Si_{0.85}Ge_{0.15}$:GaP alloy in the amplitude range of $1 \cdot 10^{-5}$–$8 \cdot 10^{-5}$, reveals a slow decrease of shear modulus and sharp increase of internal friction intensity. After achievement of $7 \cdot 10^{-4}$ amplitude of oscillatory deformation, the following measurements in the range of $5 \cdot 10^{-4}$–$5 \cdot 10^{-5}$ oscillatory deformation at amplitude decrease have revealed internal friction hysteretic change (Fig. 2).

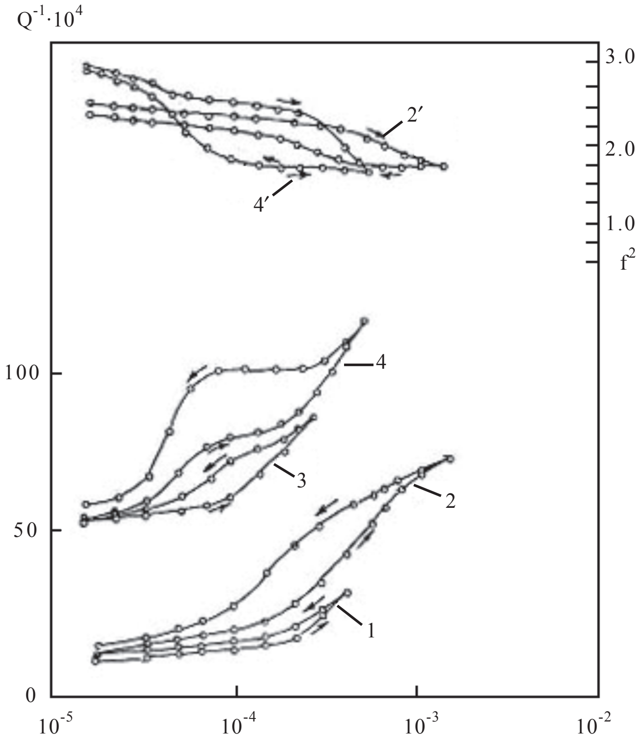

Fig. 2. Amplitude dependence of internal friction (1,2,3,4) and shear modulus in
1, 2, 2′ – cyclic deformation, 700°C
3, 4, 4′ – one - axis pressure deformation, 700°C.

The results of internal friction amplitude dependence measurements at high temperatures (400-600°C) are practically identical with the results obtained at room temperature. The difference is that the internal friction hysteresis increases with an increase of temperature, the critical amplitude of oscillatory deformation decreases at high temperatures, at which a sharp increase of the scattering energy of oscillations begins. Annealing at 500°C for 2hrs causes dislocation pinning. Accordingly, the internal friction hysteresis decreases, completely disappearing in the low range of amplitude ($1 \cdot 10^{-5}$–$5 \cdot 10^{-5}$). The amplitude dependence internal friction of the $Si_{0.85}Ge_{0.15}$ alloy deformed by compression is of more complicated nature.

The shear modulus reveals complex dependence on the amplitude of oscillation in the deformed $Si_{0.85}Ge_{0.15}$:GaP alloy. We have studied the amplitude dependence of the torsion oscillations frequency square for cyclic deformed crystals at 700°C and for crystals that are deformed by one-axis pressure. Both types of deformation cause hysteretic change of shear modulus, at the increase and decrease of amplitude cycles. Decreased values of the shear modulus are recorded on the return amplitude dependence curve. It is supposed that as a result of deformation, the bulk of doping impurities exist in solid solution, which causes local tensile deformation in the crystal lattice of $Si_{0.85}Ge_{0.15}$:GaP alloy.

Simultaneously originated dislocations by deformation exist in completely free or weak binding areas. Both of the above-mentioned factors cause a decrease of shear modulus, which is clearly revealed on the shear modulus curve. The internal friction maximum, observed at temperatures from 300 to 800°C, are of dislocation character. They are analogous to the maxima observed in torsionally deformed fiber-type silicon single crystals [6]. They may be analyzed by the Zeeger model of nucleation of dislocation kinks [7].

Considering the peculiarities of the dislocation internal friction, we may assume that the maxima, observed in the internal friction spectrum at 390 and 470°C, are provided by migration of geometric kinks on 60° and screw dislocations, respectively, while the maxima observed at 560 and 670°C, may be attributed to the processes of nucleation and migration of double kinks on screw and 60°-dislocations in the $Si_{0.85}Ge_{0.15}$:GaP alloy.

ფიზიკა

$Si_{0,85}Ge_{0,15}$:GaP შენადნობის ფიზიკურ-მექანიკური თვისებები

გ. ბოკუჩავა*, ი. ყურაშვილი*, ე. სანაია*, გ. დარსაველიძე*

* *ფ. თავაძის მეტალურგიისა და მასალათმცოდნეობის ინსტიტუტი, თბილისი*

(წარმოდგენილია აკადემიის წევრის ი. ბარათაშვილის მიერ)

შესწავლილია გალიუმის ფოსფიდით ლეგირებული $Si_{0,85}Ge_{0,15}$ შენადნობის შინაგანი ხახუნისა და ძვრის მოდულის ტემპერატურული და ამპლიტუდური დამოკიდებულებები. გამოვლენილია დისლოკაციური წარმოშობის რელაქსაციური პროცესები. განსაზღვრულია მათი აქტივაციური მახასიათებლები. რელაქსაციური შინაგანი ხახუნის პროცესების მექანიზმები გაანალიზებულია ხრახნულ და 60°-დისლოკაციებზე გეომეტრიული და წყვილი ღუნვების მოძრაობის ასპექტში.

REFERENCES

1. *I.W. Vandersande, Ch. Wood and S. Draper*. (1987), Mat. Res. Soc. Symp. Proc., **97**: 347-352.
2. *E. Iordanishvili.* (1986), Termoelectricheskie istochniki pitanija. Moscow, p.183 (Russian).
3. *C.A. Antipov, V.I. Belyavski, A.I. Drozhzhin.* (1982), J. FTT, **24**, 11: 3268-3272 (Russian).
4. *G. Darsavelidze, T. Mkheidze, I. Kurashvili, G.Bokuchava et al.* (2006), Proceedings: XVII International Conference on Radiation Material Sciences, September, Alushta. Crimea, p.101-102 (Russian).
5. *K.W. Sprungman*, *J.G. Ritchie*. (1980), Atomic Energy of Canada Limited Report, AECL-6438.
6. *S.A. Antipov, A. Drozhzhin, A.M. Rosshchupkin.* (1985), FTT. 27, 7: 2092-2094 (Russian).
7. *A. Zeeger*. (1979), Phys.Stat. Sol. (a), 55: 457-462.

Received March, 2007