Peculiarities of Internal Friction and Shear Modulus in ^{60}Co γ-Rays Irradiated Monocrystalline SiGe Alloys

I. Kurashvili, G. Darsavelidze, T. Kimeridze, G. Chubinidze, I. Tabatadze

***Abstract*—**At present, a number of modern semiconductor devices based on SiGe alloys have been created in which the latest achievements of high technologies are used. These devices might cause significant changes to networking, computing, and space technology. In the nearest future new materials based on SiGe will be able to restrict the A^3B^5 and Si technologies and firmly establish themselves in medium frequency electronics. Effective realization of these prospects requires the solution of prediction and controlling of structural state and dynamical physical –mechanical properties of new SiGe materials. Based on these circumstances, a complex investigation of structural defects and structural-sensitive dynamic mechanical characteristics of SiGe alloys under different external impacts (deformation, radiation, thermal cycling) acquires great importance. Internal friction (IF) and shear modulus temperature and amplitude dependences of the monocrystalline boron-doped $Si_{1-x}Ge_x$($x \le 0.05$) alloys grown by Czochralski technique is studied in initial and ^{60}Co gamma-irradiated states. In the initial samples, a set of dislocation origin relaxation processes and accompanying modulus defects are revealed in a temperature interval of 400-800 ^{0}C. It is shown that after gamma-irradiation intensity of relaxation internal friction in the vicinity of 280 ^{0}C increases and simultaneously activation parameters of high temperature relaxation processes reveal clear rising. It is proposed that these changes of dynamical mechanical characteristics might be caused by a decrease of the dislocation mobility in the Cottrell atmosphere enriched by the radiation defects.

***Keywords*—**Gamma-irradiation, internal friction, shear modulus, SiGe alloys.

I. Introduction

THE investigation of defects in SiGe alloys' bulk crystals might be successfully carried out by the IF method, which is distinguished by high sensitivity to the mechanical stress field formed in the vicinity of crystalline lattice defects. It makes possible to effectively identify defects of SiGe alloys bulk crystals, to establish mechanisms of their influence on the structural sensitive physical-mechanical and electrophysical properties. Such research will help to solve the problem of creating highly efficient semiconductor structures and devices with controllable parameters based on SiGe alloys.

The contribution of a dislocation structure in relaxation and hysteretic processes of torsion oscillations damping in SiGe alloys' bulk crystals has been studied [1]-[3]. Decrease of the activation characteristics of relaxation processes of dislocation origin is shown by influence of a relatively small content of Ge (1-3 at%). Reduction by ~15% in the microplastic deformation characteristics has been revealed at 600-650 ^{0}C temperatures in $Si_{1-x}Ge_x$ ($x \le 0.02$) alloys containing dislocations of 10^4-10^5 cm^{-2} densities [1]. An additional reduction of IF activation characteristics has been revealed in $Si_{1-x}Ge_x$($x \le 0.01$) alloys doped with As or B of 10^{18}-10^{20} cm^3 concentration [4]. SiGe alloys are characterized by different types of dislocations with distinctly different energetic and dynamic parameters [5]-[7]. This conditions the formation of complex IF spectra related to the moving dislocations.

Relaxation maximum with activation energy ~1.4 eV was revealed at 280 °C temperature at ~1 Hz frequency in IF spectrum of p-type monocrystalline $Si_{0.98}Ge_{0.02}$ irradiated by gamma rays. Its relation to the radiation-induced vacancy-oxygen complexes is supposed [3].

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II. Methodology

SiGe bulk crystals were grown by the Czochralski technique in argon atmosphere. Seeds of Si single crystal with [111] orientation were used for the growth of the SiGe crystals. Microstructure was investigated on the optical microscope NMM-80RF/TRF. Electrophysical characteristics were determined in the constant magnetic field of 0.5 Tesla induction on the Ecopia HMS-3000 device by Hall effect measurements.

Investigations of the internal friction and shear modulus were carried out on the vacuum device by registration of logarithmic decrement of damping and frequency of the reverse pendulum free torsion oscillations in the ranges of 20-800 ^{0}C temperature, 0.5-5.0 Hz frequency and 10^{-5}-10^{-3} strain amplitude.

SiGe samples of [$\bar{2}$11] orientation and 0.8 mm x 0.8 mm x 30-35 mm sizes were used for investigating dynamic mechanical properties.

The activation energy of relaxation IF maxima was determined by the formula [8]:

$$H = R \cdot \left(\frac{1}{T_1} - \frac{1}{T_2} \right) \ln \frac{f_2}{f_1} \quad (1)$$

where R is the gas constant, T_1, T_2 are the temperatures of maxima at f_1 and f_2 frequencies.

The values of frequency factor $\frac{1}{\tau_0}$ were determined from the known equation $\omega_{max.} \cdot \tau = 1$, where and $\omega_{max.} = 2\pi \cdot f_{max}$ and $\tau = \tau_0 \cdot \exp\left(\frac{H}{RT_{max}}\right)$

Rotation angle of sample edge was considered as torsion deformation, from which the value of strain amplitude was determined by the following equation:

$$\varepsilon = \frac{r \cdot L}{l \cdot R} \tag{2}$$

where r is the radius of circumscribed circle around quadratic cross-section of parallelepiped shaped specimens, l is the length of the specimen, R is the distance between the sample and registration scale, L is the deviation of reflected ray from a mirror fixed on the specimen.

III. Results and Analysis

Microstructure of boron doped $Si_{1-x}Ge_x$ ($x \le 0.05$) alloys on the (111) planes is characterized by a non-uniform distribution of dislocation etch pits. The dislocation density is increased with increase of Ge content. Dislocation groups are often fixed in the microstructure of the alloys with $x \ge 0.03$. The changes of density and distribution of dislocations in the microstructure of the gamma-irradiated samples have not been practically revealed. Dislocation density in the initial as well as irradiate specimens varies in a range of $1\cdot10^4$-$1\cdot10^5$ cm^{-2}.

All samples in the initial state are characterized by p-type conductivity, low concentration and mobility of current carriers.

Thermal annealing at temperatures of 300-400 ^{0}C in vacuum does not affect the electrophysical characteristics of non-irradiated Si, $Si_{0.99}Ge_{0.01}$ and $Si_{0.97}Ge_{0.03}$ samples. $Si_{0.96}Ge_{0.04}$ sample in annealed state is characterized by a weak increase of hole mobility. This is conditioned by annihilation of electrically active technological defects distributed in stress fields near the Ge atoms and in the impurity atmosphere around dislocations (Table I).

TABLE I
ELECTROPHYSICAL CHARACTERISTICS OF MONOCRYSTALLINE SI AND SIGE ALLOYS

Samples	Current Carriers Concentration, cm^{-3}			Current Carriers Mobility, cm^{2}v^{-1}s^{-1}		
	Initial state	Gamma irradiated state	Annealed at 300 ^{0}C, 1 h.	Initial state	Gamma irradiated state	Annealed at 300^{0}C, 1h.
Si:B	$7\cdot10^{13}$	$1\cdot10^{14}$	$6\cdot10^{13}$	430	400	440
$Si_{0.99}Ge_{0.01}$:B	$8\cdot10^{13}$	$2\cdot10^{14}$	$7\cdot10^{13}$	410	370	420
$Si_{0.97}Ge_{0.03}$:B	$5\cdot10^{13}$	$5\cdot10^{13}$	$2\cdot10^{13}$	425	380	435
$Si_{0.96}Ge_{0.04}$:B	$5\cdot10^{13}$	$8\cdot10^{13}$	$4\cdot10^{13}$	450	390	460

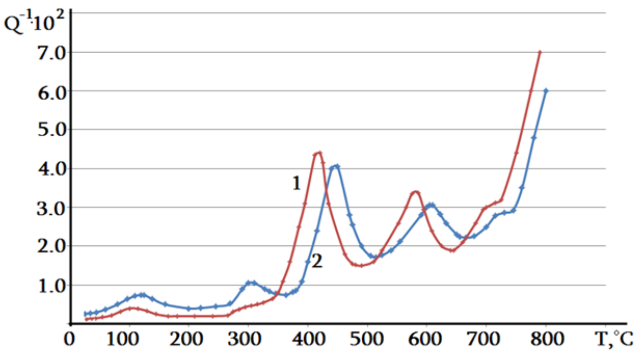


Fig. 1 Temperature dependence of internal friction of monocrystalline Si of [111] orientation; 1. Initial state, f_0=1.2 Hz; 2. after gamma-irradiation, f_0=1.1 Hz

In gamma-irradiated samples, a significant increase in current carriers' concentration and their mobility reduction are revealed. Such changes are conditioned by the point defects and their simple complexes formed by irradiation. Thermal annealing (300 °C, 1h) of all the samples irradiated with gamma-rays causes a reduction in the concentration of holes and an increase in their mobility to the initial level. Obviously, the annealing causes transformations in the structure of radiation defects and a reduction in the concentrations of electrically active defects.

The IF temperature spectrum of monocrystalline Si of [111] orientation is characterized by wide maxima in the 100-800 ^{0}C temperature range (Fig. 1).

Shapes of the IF maxima are distorted by their overlapping and exponentially growing background. The intensity of the IF background and maxima in 400-800 ^{0}C temperature range significantly increase at high strain amplitudes of 10^{-4}-10^{-3}. This circumstance reveals their dislocation nature.

All IF maxima change their critical temperature by changing oscillations frequency. According to the well-known theory [8], they are of relaxation origin. This is also confirmed by revealing the shear modulus defects being proportional to the maxima intensity (Fig. 2).

The values of activation energy and frequency factors are presented in Table II. Irradiation of monocrystalline Si by gamma-rays stipulates an increase in the IF intensity at 100 and 280 ºC and a weak rise in the critical temperatures of relaxation maxima in the 400-800 ºC temperature range. Gamma irradiation of monocrystalline Si causes a rise in the activation characteristics of high-temperature relaxation processes in comparison with identical values of Si in the initial state. Thermal annealing at 600 ºC for 3 h of gamma-irradiated samples of Si completely suppresses the IF maxima at 100 and 280 ºC temperatures. In the annealed state, the IF exponential background shifts towards high temperatures.

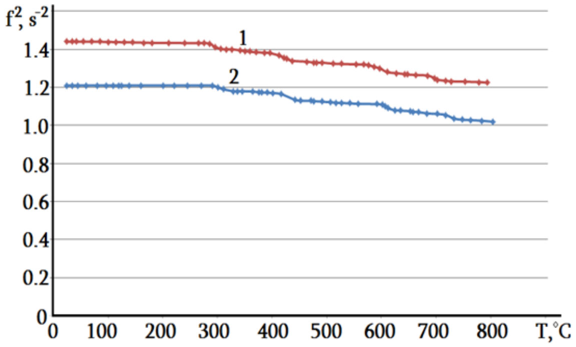


Fig. 2 Temperature dependence of shear modulus of monocrystalline Si of [111] orientation; 1. Initial state, f_0=1.2 Hz; 2. after gamma-irradiation, f_0=1.1 Hz

The following peculiarities have been revealed in the IF temperature spectra of the monocrystalline SiGe alloys irradiated by gamma rays (Fig. 3).

An increase in the content of Ge stipulates a reduction in the intensity of IF maxima at 100 and 280 ^{0}C temperatures; however, their activation characteristics remain unchanged in comparison with the identical values in nonirradiated states. The IF maxima revealed in the 400-800 ^{0}C range are shifting by 15-20 ^{0}C towards high temperatures. Respectively, an increase in the activation characteristics is clearly shown (see Table II).

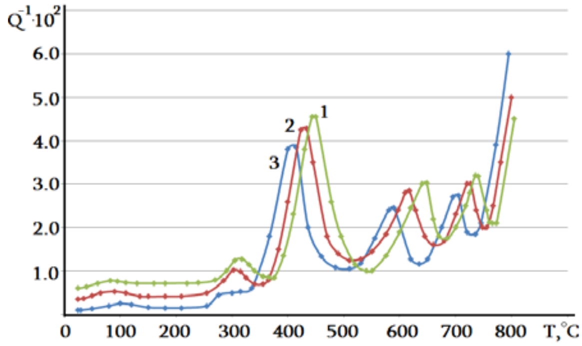


Fig. 3 Temperature dependence of internal friction of monocrsyatlline SiGe alloys after gamma irradiation; 1. $Si_{0.99}Ge_{0.01}$, f_0=1.8 Hz; 2. $Si_{0.97}Ge_{0.03}$, f_0=2.0 Hz; 3. $Si_{0.96}Ge_{0.04}$, f_0=2.15 Hz

TABLE II
ACTIVATION CHARACTERISTICS OF INTERNAL FRICTION RELAXATION MAXIMA

Samples	Temperature of IF maxima, ºC		Activation energy, eV		Frequency factor, s^{-1}	
	Initial state	After gamma irradiation	Initial state	After gamma irradiation	Initial state	After gamma irradiation
Si:B	-	100	-	0.90	-	$6.5\cdot10^{12}$
	280	300	1.35	1.40	$1\cdot10^{13}$	$2\cdot10^{13}$
	410	420	1.50	1.60	$6\cdot10^{11}$	$2\cdot10^{12}$
	600	615	1.65	1.80	$2\cdot10^{10}$	$6\cdot10^{10}$
	710	725	2.10	2.20	$3.5\cdot10^{11}$	$6.3\cdot10^{11}$
$Si_{0.99}Ge_{0.01}$:B	100	100	-	0.90	-	$6\cdot10^{12}$
	280	300	1.30	1.50	$3.5.10^{12}$	$6.3\cdot10^{13}$
	400	415	1.60	1.75	$4.4\cdot10^{12}$	$3.4\cdot10^{13}$
	590	600	1.70	1.80	$6\cdot10^{10}$	$2\cdot10^{11}$
	700	720	2.00	2.10	$1.5\cdot10^{11}$	$2\cdot10^{11}$
$Si_{0.97}Ge_{0.03}$:B	100	100	0.9	0.9	$5\cdot10^{12}$	$5\cdot10^{12}$
	285	285	1.3	1.3	$4\cdot10^{12}$	$8\cdot10^{12}$
	400	405	1.6	1.65	$6\cdot10^{12}$	$7.5\cdot10^{12}$
	590	600	1.7	1.75	$8\cdot10^{11}$	$1\cdot10^{12}$
	690	700	1.8	1.85	$6\cdot10^{11}$	$8.5\cdot10^{11}$
$Si_{0.96}Ge_{0.04}$:B	100	100	0.90	0.90	$1\cdot10^{13}$	$1\cdot10^{13}$
	280	290	1.30	1.45	$3.5.10^{13}$	$5\cdot10^{13}$
	390	400	1.65	1.70	$2\cdot10^{13}$	$2.2\cdot10^{13}$
	600	605	1.65	1.75	$3\cdot10^{10}$	$7\cdot10^{10}$
	685	700	1.90	2.00	$6\cdot10^{10}$	$1.7\cdot10^{11}$

Fig. 4 shows temperature changes of shear modulus of gamma-irradiated SiGe alloys. At the critical temperatures, the shear modulus defect is revealed in proportion to the relaxation process intensity. Annealing at 600 ^{0}C for 3 h in vacuum of SiGe samples causes a sharp reduction in the intensity of the IF maxima at 100 and 280 ^{0}C and a slight decrease in the other maxima intensity. A weak reduction of the shear modulus is revealed at critical temperatures.

High-temperature cyclic deformation of SiGe samples at 600 ^{0}C stipulates a noticeable increase in the relaxation maxima intensity in the 400-800 ^{0}C range and a reduction in their critical temperatures. Consequently, the shear modulus defects increase at the critical temperatures. It should be noted that activation characteristics of the relaxation maxima at 100 and 280 ^{0}C temperatures are independent from high-temperature cyclic deformation. Thermal annealing at ≈ 600 ^{0}C for 3 h after high-temperature cyclic deformation causes complete suppression of maximum near 100 ^{0}C and a sharp reduction in the relaxation process intensity in the vicinity of 280 ^{0}C.

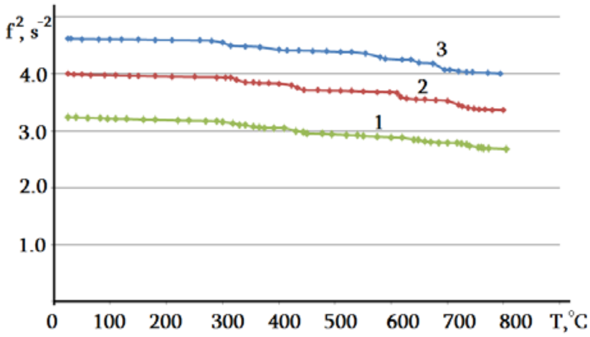
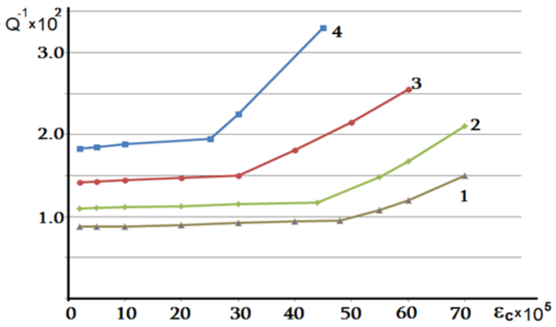
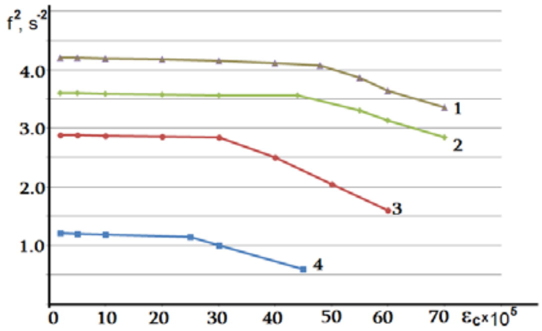


Fig. 4 Temperature dependence of shear modulus of monocrsyatlline SiGe alloys after gamma irradiation; 1. $Si_{0.99}Ge_{0.01}$, f_0=1.8 Hz; 2. $Si_{0.97}Ge_{0.03}$, f_0=2.0 Hz; 3. $Si_{0.96}Ge_{0.04}$, f_0=2.15 Hz;



(a)



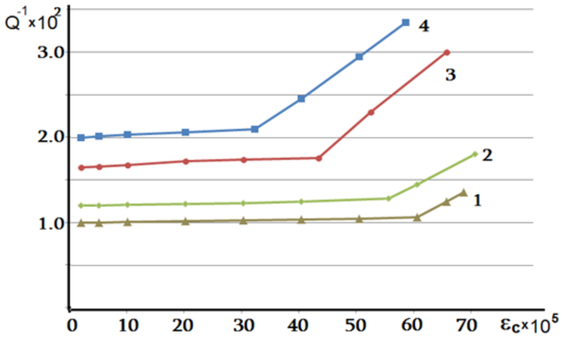
(b)

Fig. 5 Amplitude dependence of IF (a) and shear modulus (b) of monocrystalline SiGe alloys in initial states; 1. Si; 2. $Si_{0.99}Ge_{0.01}$; 3. $Si_{0.97}Ge0_{.03}$; 4. $Si_{0.96}Ge_{0.04}$

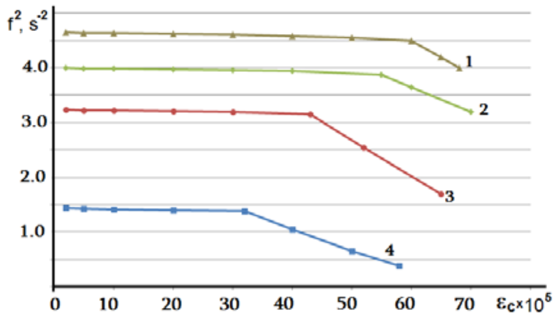
At room temperature all the experimental specimens are characterized with low background of IF (max. strain amplitude- $5{\cdot}10^{-3}$, number of cycles -500) in a wide range of torsion oscillation amplitudes and with first critical strain amplitude (ε_c), from which slight linear increase of $Q^{-1}(\varepsilon)$ is revealed (Fig. 5). The tendency to decrease the first critical strain amplitude (ε_c) is observed. For all the experimental specimens in a wide range of strain amplitudes ascending and descending branches of $Q^{-1}(\varepsilon)$ curves coincide with each other. Therefore, at the room temperature bulk crystals of Si-Ge alloys with low Ge content practically do not reveal plastic deformation in the range of 10^{-5}-5.10^{-3} torsion oscillation amplitudes.

Figs. 5 (a) and (b) show that an increase of Ge content stipulates reduction of the values of strain amplitude. Obviously this circumstance is related to the local deformations formed near Ge atoms with large atomic radius in the crystalline lattice of SiGe alloys.

After gamma irradiation, all specimens are characterized by significantly high values of strain amplitude Fig. 6 (a,b). This indicates that there is a radiation hardening of the experimental samples.



(a)



(b)

Fig. 6 Amplitude dependence of IF (a) and shear modulus (b) of monocrystalline SiGe alloys after gamma-irradiation; 1. Si; 2. $Si_{0.99}Ge_{0.01}$; 3. $Si_{0.97}Ge0_{.03}$; 4. $Si_{0.96}Ge_{0.04}$

It is proposed that radiation hardening is a result of reduction of dislocation mobility in a process of gamma radiation, due to an increase of pinning centers concentration in Cottrell's atmosphere and in the vicinity of dislocation nuclei.

TABLE III
INFLUENCE OF GAMMA IRRADIATION ON THE CRITICAL STRAIN AMPLITUDE OF SIGE: B MONOCRYSTALS

Materials	Critical Strain Amplitude, $x10^5$		Dislocation Density, cm^{-2}	
	Initial state	Gamma irradiated state	Initial state	Gamma irradiated state
Si:B	50	60	$2{\cdot}10^4$	$3{\cdot}10^4$
$Si_{0.99}Ge_{0.01}$:B	45	55	$4{\cdot}10^4$	$5{\cdot}10^4$
$Si_{0.97}Ge_{0.03}$:B	30	45	$7{\cdot}10^4$	$7{\cdot}10^4$
$Si_{0.96}Ge_{0.04}$:B	25	32	$1{\cdot}10^5$	$1{\cdot}10^4$

IV. Conclusion

Increase of activation characteristics of dislocation IF processes and the values of critical strain amplitude, at which break-away of dislocations from pinning points takes place, were revealed in monocrystalline $Si_{1-x}Ge_x(x \leq 0.05)$ alloys irradiated by gamma rays of fluence $\sim 10^{17} cm^{-2}$.

Acknowledgment

This work was supported by Shota Rustaveli National Science Foundation (SRNSFG) [#217562. Peculiarities of internal friction spectra and microhardness of SiGe monocrystals].

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