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Physical-Mechanical Characteristics of Monocrystalline $Si_{1-x}Ge_x$ ($x \leq 0,02$) Solid Solutions

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***Abstract*—**Si-Ge solid solutions (bulk poly- and mono-crystalline samples, thin films) are characterized by high perspectives for application in semiconductor devices, in particular, optoelectronics and microelectronics. From this point of view, complex studying of structural state of the defects and structural-sensitive physical properties of Si-Ge solid solutions depending on the contents of Si and Ge components is very important. Present work deals with the investigations of microstructure, microhardness, internal friction and shear modulus of Si1-xGex(x≤0,02) bulk monocrystals conducted at room temperature. Si-Ge bulk crystals were obtained by Czochralski method in [111] crystallographic direction. Investigated monocrystalline Si-Ge samples are characterized by p-type conductivity and carriers' concentration $5\cdot10^{14}$-$1.10^{15}cm^{-3}$. Microhardness was studied on Dynamic Ultra Micro hardness Tester DUH-201S with Berkovich indenter.

Investigate samples are characterized with 0,5x0,5x(10-15)mm3 sizes, oriented along [111] direction at torsion oscillations ≈1Hz, multistage changing of internal friction and shear modulus has been revealed in an interval of strain amplitude of 10^{-5}-5.10^{-3}. Critical values of strain amplitude have been determined at which hysteretic changes of inelastic characteristics and microplasticity are observed.

The critical strain amplitude and elasticity limit values are also determined. Dynamic mechanical characteristics decreasing trend is shown with increasing Ge content in Si-Ge solid solutions. Observed changes are discussed from the point of view of interaction of various dislocations with point defects and their complexes in a real structure of Si-Ge solid solutions.

***Keywords*—**Internal friction, microhardness, relaxation processes, shear modulus, Si-Ge.

I. Introduction

It is well known that in Si-Ge crystalline lattice Ge atoms can strongly interact with intrinsic point defects, i.e. vacancies and self-interstitials, because of elastic strains in the crystal lattice related to the mismatch of their atomic size as compared to that of host atoms. This property of isovalent atoms can be used to modify interactions of point defects and dislocations during crystal growth as well as under irradiation and annealing [1].

In difference from silicon regularities of structural defects formation and motion, structural-sensitive properties of volume Si-Ge crystals are little studied. Until today the problems of obtaining perfect homogeneous Si-Ge crystals with predetermined real structure and properties have not been solved.

Recent studies show great potential for modification electrophysical and mechanical properties and radiation resistance of silicon during Ge doping. [1]-[3]. Complex character of mechanical properties changes, depending on Ge content in Si-Ge alloys has been shown. [4]-[6]. Regularities of influence of defects characteristics on dynamic mechanical properties of Si-Ge crystals have been revealed [7].

Present work deals with investigations of temperature spectra of internal friction and dynamic shear modulus, defects characteristics, participant in relaxation energy dissipation, mechanical oscillations and nonmonotonous changes of shear modulus in Si-Ge alloys. Dynamic microhardness and indentation modulus have been investigated in a wide range of penetration depth of Berkovich indenter in Si-Ge monocrystals.

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II. Experiment

Internal friction (Q-1) and squared frequency (f2), proportional to the dynamic shear modulus, were investigated by the laboratory equipment with reverse torsion pendulum, on which axis samples with 0,6-0,8mm diameter and 40-50mm length were fixed with refractory clay based on SiO2. Measurements of Q-1 and f2 temperature dependences were carried out in vacuum 10-4 Torr. Sample temperature, logarithmic decrement of damping and oscillations frequency were determined semi-automatically. Annealing-cooling velocity varied in 1-3°C/min interval, oscillations frequency in 0,5-5,0Hz, strain amplitude in 1.10-5-5.10-3 range and temperature in 20-950°C interval. Heating was carried out indirectly by a resistance furnace.

Activation characteristics of relaxation processes have been determined by known Wert-Marx equation [8]:

$$H \approx R \cdot T_{\max} \cdot \ln \frac{R \cdot T_{\max.}}{h \cdot f_{\max}}$$

where R-gas constant, h- Planck's constant, Tmax and fmax temperature and frequency of maxima.

The absolute value of shear modulus is calculated at the room temperatures by comparing the standard and test specimens [9]:

$$G = G_0 \cdot \left(f^2 / f_o^2 \right)$$

where G_0 and f_0 are shear modulus and oscillation frequency of the standard specimens (V, W), and G and f - shear modulus and oscillation frequency of the test specimen. Frequency measurements of the specimens with identical sizes and shapes were carried out on internal friction device.

Studying of microhardness and indentation modulus of Si-Ge alloys was carried out by on Dynamic Ultra Micro hardness Tester DUH-201S with Berkovich indenter. Indentation testing was performed in load-unload mode for different loadings in range 2 to 900 mN. Hold time at load 10[sec]/ Hold time at unload 5[sec]. Penetration depth of indenter in material increased proportional to the loading value. Values of the microhardness measurement errors in interval of high loads 200 to 1,000 mN do not exceed 3% and one order of magnitude higher for small loads.

III. Results and Discussions

Temperature dependences of internal friction and dynamic shear modulus of p- type Si + 0,5at% Ge, Si + 1,2at% Ge and Si + 1,2at% Ge alloys have been studied. Samples were oriented in [111] crystallographic direction. Dislocation density in their real structure has been varied within 103-104cm -2.

Fig. 1 shows internal friction spectra of Si-Ge alloys; those contain intensive maxima on exponential background in 300, 450,600 and 720°C temperatures areas.

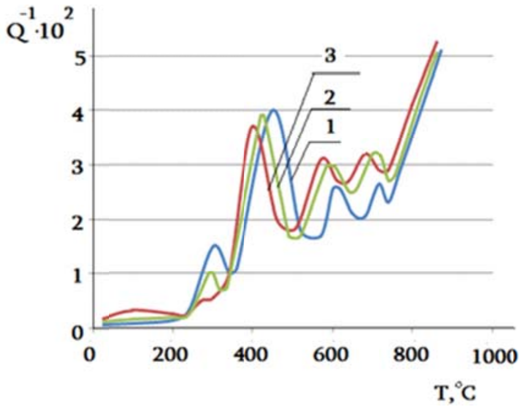


Fig. 1 Internal friction temperature spectra of monocrystalline Si-Ge alloys 1. Si+0,5at%Ge, 2. Si+1,2at%Ge, 3. Si+2at%Ge

During the first measurement intensities of background and all Q-1 maxima significantly decrease under the influence of heating. In this condition by increase of oscillations frequency up to 5Hz maxima shift towards high temperatures by 15-20°C It confirms relaxation nature of internal friction maxima. Besides, maxima in 450, 600 and 720°C temperatures area are characterized with raising of intensity by increasing strain amplitude in 10-4-5.10-3 interval. According to the theory [8] such type of relaxation maxima are deformation origin and in formation of them dislocations take place. Relaxation maxima activation characteristics are presented in Table I.

Nonmonotonous changes of shear modulus in a wide temperature interval confirm complicated nature of torsion oscillations energy scattering processes (Fig. 2).

TABLE I
Relaxation Processes Activation Characteristics of Monocrystalline SI_GE Alloys

Samples	Temperatures of maxima, °C	Activation characteristics, eV
Si+0,5 at %Ge	300	1,35
	450	1,70
	600	1,95
	720	2,30
Si+1,2 at %Ge	300	1,30
	430	1,60
	585	1,85
	710	2,15
Si+2 at %Ge	300	1,30
	410	1,60
	570	1,80
	680	2,00

At the relaxation processes temperatures shear modulus defect (sharp decrease) has been revealed. Its value is proportional to the relaxation maxima intensity. The known equation is fulfilled for all relaxation maxima [8]:

$$\Delta G / G = 2 \cdot Q^{-1}_{\max}.$$

where ΔG/G – modulus defect, Q-1max – internal friction maxima intensity.

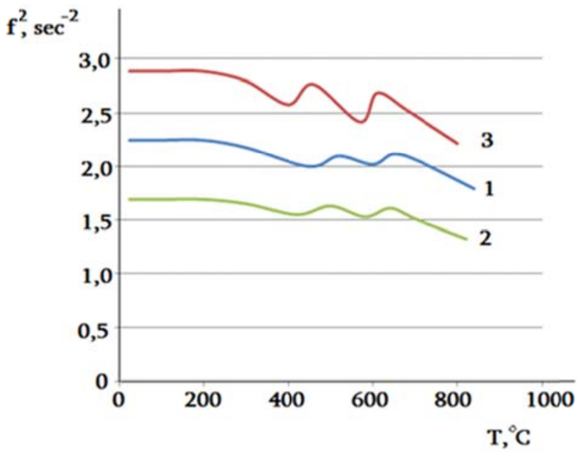


Fig. 2 Temperature dependence of squared frequencies, proportional to shear modulus of monocrystalline Si-Ge alloys 1. Si+0,5at%Ge, 2. Si+1,2at%Ge, 3. Si+2at%Ge

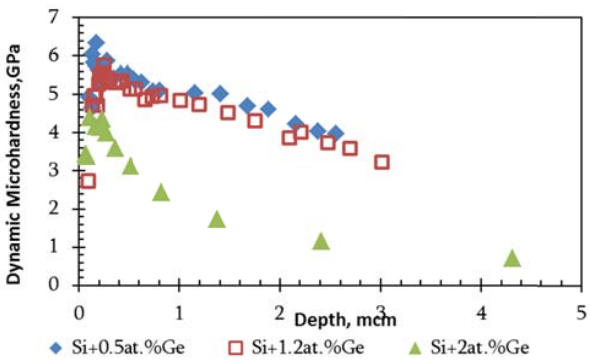
As is established from Fig. 2 temperature intervals of shear modulus anomalous increasing have been revealed. They shift towards low temperatures. At the same time shear modulus anomalies reveal more clearly with increasing Ge concentration in Si-Ge alloys.

Thermal annealing in vacuum at 800°C temperature for 5 hrs. causes significant decrease of relaxation internal friction maxima intensities and reveals tendency to their shifting towards high temperatures. In abovementioned conditions thermal annealing practically does not influence on nonmonotonous variation of shear modulus. It is supposed, that shear modulus anomalous changes in a wide range of temperature may be connected to the configuration and composition transformation in various defects complexes distributed in the Cottrell atmosphere of dislocations.

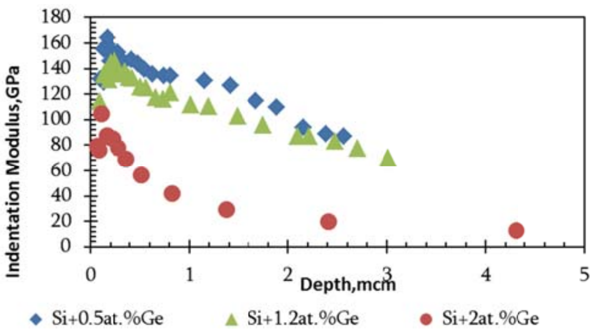
Shear modulus absolute values of Si-Ge samples have been decreased by increasing Ge concentration in Si-Ge alloys. Annealing at 800°C for 10hrs stipulates increase of shear modulus absolute value.

Decrease of activation energy of dislocation origin relaxation maxima by increasing Ge concentration is in full compliance with literature data [5], where based on σ-ε diagrams analysis, raising different types dislocations mobility has been shown in a wide range of Ge concentration in bulk Si-Ge alloys.

It is presented changes of dynamic microhardness and indentation modulus (Figs. 3 (a), (b)) in a wide range of Berkovich indenter penetration on the [111] planes of monocrystalline substrates with different Ge concentration. Both mechanical characteristics have changed nonmonotonously in surface layers and reverse Indentation Size Effect (ISE) has been revealed.



(a)



(b)

Fig. 3 Dynamic microhardness (a) and indentation modulus (b) versus penetration depth in Si-Ge alloys for different Ge concentration

In Table II maximal values of Berkovich dynamic microhardness and indentation modulus of monocrystalline Si-Ge substrates in reverse ISE area have been presented. It is established, that maximum values of dynamic microhardness and indentation modulus of Si+0,5at.%Ge and Si+1.2at.%Ge alloys have been revealed at the same penetration depth. Unlike them, in Si+2at.%Ge substrate maximal values of dynamic microhardness and indentation modulus have been observed at the two different penetration depth, 0.232 and 0.108, respectively.

TABLE II
MAXIMAL VALUES OF DYNAMIC MICROHARDNESS AND INDENTATION MODULUS IN ISE AREA

Ge content, at%	hmax, μm	Dynamic microhardness, GPa	Indentation modulus, GPa
0,5	0.1757	6.331	164.3
1,2	0.2477	5.77	145.5
2,0	0.232/0.108	4.361	104.5

At high values of indenter penetration depth dynamic microhardness and indentation modulus are determined mainly in volume structural state. In abovementioned condition tendency to decreasing mechanical characteristics is stipulated by increasing Ge concentration. Stresses localized near Ge atoms with high atomic radius weaken interatomic bonding forces, those are the main reason of decreasing dynamic microhardness and indentation modulus of the alloys. Annealing in vacuum at 850°C temperature for 10 hrs. stipulates weak increase of dynamic microhardness and indentation modulus. Annealing in high penetration depth also slightly reduces ISE of microhardness and indentation modulus

IV. CONCLUSIONS

Increase of Ge concentration in Si-Ge alloys causes decrease of dislocation origin relaxation processes' activation energies and shear modulus anomalous changes. Reverse ISE is shown. Maximal values of dynamic microhardness and indentation modulus decrease under increase of Ge concentration in investigated specimens. Weakening of interatomic bonding forces and distortion of lattice caused by Ge atoms, stipulate decrease of activation characteristic of dislocation relaxation processes, dynamic microhardness and elastic modulus in bulk alloys.

Microscopic mechanisms of dynamic mechanical characteristics changing in bulk Si-Ge monocrystalline alloys is subject of our further investigations.

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