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INFLUENCE OF GERMANIUM AND BORON DOPING ON STRUCTURAL AND PHYSICAL_MECHANICAL CHARACTERISTICS OF MONOCRYSTALLINE SILICON

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Abstract

Complex studying of microstructure, electrophysical characteristics and internal friction and shear modulus temperature spectra of monocrystalline Si-Ge-B alloys during torsion oscillations of 1Hz frequency were conducted. Boron doped $Si_{1-x}Ge_x$ ($x<0,03$) bulk monocrystals with [111] orientation were obtained by the Czochralski method. Regularities of changing of density and character of dislocation distribution on (111) planes, concentration and mobility of current carriers, activation characteristics of relaxation internal friction maximum were established. Establishment of correlation between their real structure, electrophysical and structural-sensitive physical-mechanical characteristics is important for broadening of practical application areas of Si-Ge bulk crystals. From this point of view in the present work microstructure, electrophysical characteristics, shear modulus and internal friction temperature spectra of Si Ge alloys depending on boron doping level have been studied. The contribution of various dislocations in variations of dynamical mechanical characteristics and relaxation internal friction in Si-Ge alloys have been discussed.

Key words: *Silicon, germanium, boron, activation energy, internal friction, shear modulus.*

1. INTRODUCTION

Germanium –doped monocrystalline silicon are of great interest for their practical applications in microelectronics and optoelectronics apparatus, in X-ray monochromators, neutron and X-ray detectors. There is possible to change smoothly the forbidden gap width and crystal lattice parameters in Si-Ge alloys by Ge content variation. This has a great importance for the development of the various semiconductor devices with defined characteristics. Actuality of complex studying of bulk monocrystalline Si-Ge alloys structure, electrophysical and physical-mechanical properties is stipulated by their wide application possibilities in electronic and optoelectronic devices.

At present, crystallographic and energetic characteristics of dislocation origin defects in monocrystalline Si-Ge alloys structure, as well as thermal stability and electrical activity of various structural defects is not practically studied. Sustainability of Si-Ge alloys real structural state and structural-sensitive physical –mechanical properties to thermal, mechanical and radiation influences is not sufficiently investigated.

The purpose of the work is the complex investigation of microstructure, electrophysical and physical-mechanical properties of boron and germanium doped monocrystalline silicon and establishment of changing regularities of the above mentioned properties by doping, thermal and mechanical treatments.

It is well known, that in the process of cutting and mechanical polishing in the surface structure of Si substrates high concentration point defects and their clusters, and dislocation origin defects have been formed. They determined instability of structural-sensitive mechanical and electrophysical characteristics under thermal, deformation and radiation influence.

Estimation of various deformation defects contribution in changing of structural-sensitive properties of the semiconducting Si-Ge substrates is possible by complex studying of microstructure, electrophysical characteristics and lowtemperature internal friction spectra.

2. EXPERIMENTAL

Present work deals with investigations of structural-sensitive physical-mechanical properties of the undoped and boron and germanium doped silicon. Experimental samples were obtained by Czochralski method in the inductive heating furnace of EQ-SKJ-50CZ system in argon atmosphere along [111] crystallographic direction. For the microstructural analysis (111) planes of experimental specimens were prepared by standard methods. At

the last stage of mechanical treatment specimens were polished by 0,25 μm grain sizes diamond pastes. After this microstructure was revealed by chemical polishing and etching. Microstructure of the experimental samples was investigated by the optical microscope NMM-800RF/TRF. Electrophysical characteristics were determined in the constant magnetic field of 0,5 Tesla induction on the Ecopia HMS3000 device by the Hall effect measurements. Investigations of internal friction and relative shear modulus were conducted on the laboratory device by registration of logarithmic decrement of torsion oscillations damping in the frequency range of 0,5-5,0Hz.

3. RESULTS AND DISCUSSION

In the microstructure of Si-Ge monocrystals on (111) plane inhomogeneously distributed dislocations are revealed. Their density varies in the range of 1.103- $1 \cdot 10^4 cm^{-2}$. In the microstructure of boron doped Si-Ge specimens number of etch pits is relatively higher. In the microstructure of $Si_{0,98}Ge_{0,02}$:B (~$10^{18} cm^{-3}$) monocrystal deformation lines are revealed, which contain etch pits. High dislocation density and their inhomogeneous distribution stipulated by inhomogeneous deformation is characteristic for Si-Ge monocrystals with high content of germanium and boron. Investigations results of microstructure of Si-Ge alloys with different content are presented on figure 1.

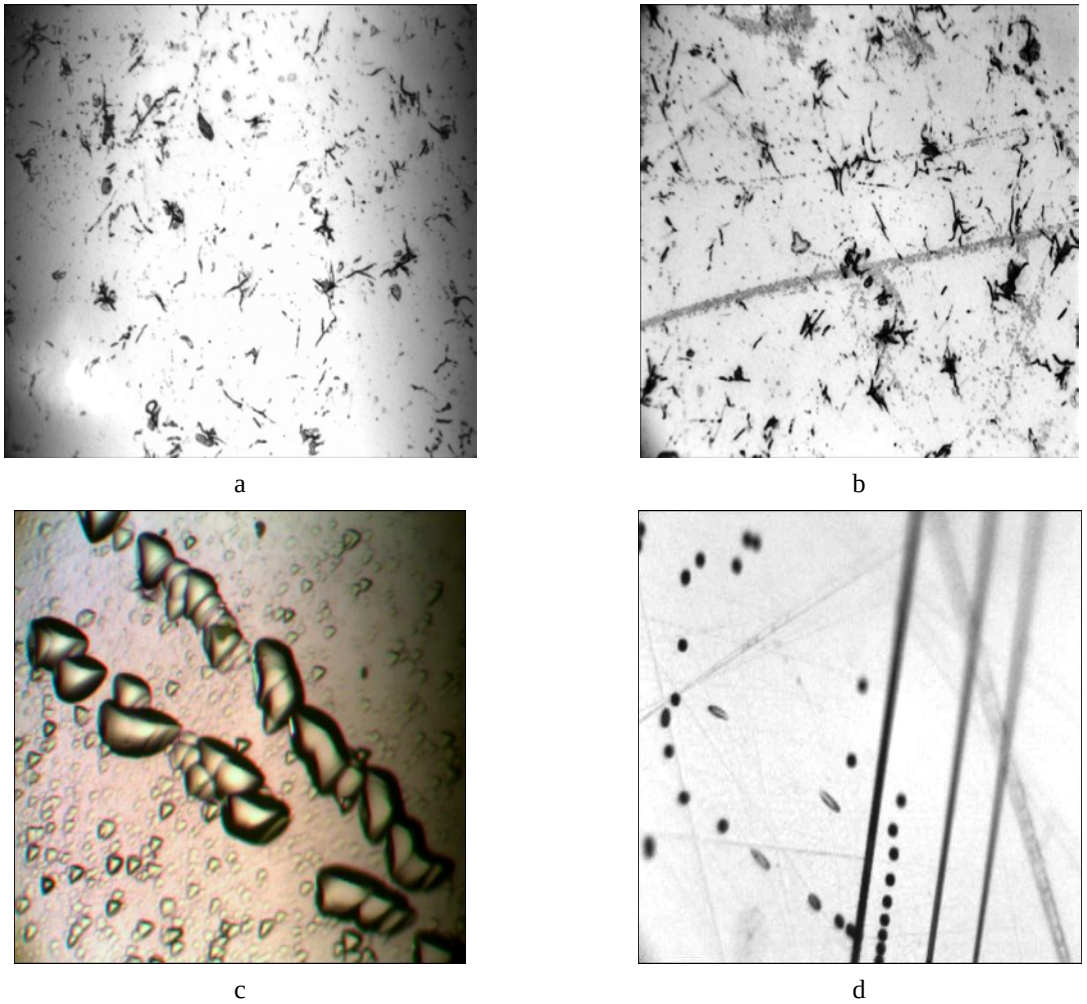

Fig.1. Microstructures of Si-Ge alloys on the (111) planes
a -Si+2,2at.%Ge b -Si+2,2at.%Ge:B ($10^{14} cm^{-3}$) c -Si+2,2at.%Ge:B ($10^{16} cm^{-3}$)
c -Si+2,2at.%Ge:B ($10^{16} cm^{-3}$)

In the internal friction temperature spectrum of Si+ 0,5 at.% Ge monocrystals with [111] direction in the vicinity of -50°C temperature at 0,8 Hz frequency of torsion oscillation, wide maximum has been revealed. Intensity of background of vibration energy scattering is practically independent on the temperature. By increasing oscillation frequency from 0,5 up to 5,0 Hz maximum has shifted towards high temperatures. According to the theory this kind of maxima are relaxation origin. The values of activation energy and frequency factor of relaxation processes are determined on the basis of internal friction maximum shifting along temperature axis [1]. Relaxation processes activation characteristics are presented in the table 1.

Table 1. Physical-mechanical characteristics of monocrystalline Si-Ge alloys

Experimental specimens	Dislocation density, cm^{-2}	Current carriers concentration, cm^{-3}	Temperature of relaxation maximum, ^0C	Activation energy , eV	Frequency factor, sec^{-1}
Si+0,5at.%Ge	$2 \cdot 10^3$	$1 \cdot 10^{12}$	-50	0,5	$6 \cdot 10^{11}$
Si+0,5at.%Ge:B	$5 \cdot 10^3$	$3 \cdot 10^{12}$	-42	0,55-0,6	$5 \cdot 10^{12}$
Si+0,5at.%Ge:B	$1 \cdot 10^{14}$	$1 \cdot 10^{18}$	-60	0,4	$3 \cdot 10^{11}$
Si+1,6at.%Ge	$5 \cdot 10^3$	$5 \cdot 10^{12}$	-55	0,45	$2 \cdot 10^{11}$
Si+1,6at.%Ge :B	$5 \cdot 10^3$	$8 \cdot 10^{14}$	-52	0,48-0,50	$7 \cdot 10^{11}$
Si+1,6at.%Ge :B	$8 \cdot 10^3$	$5 \cdot 10^{18}$	-65	0,35	$1 \cdot 10^{10}$
Si+2,2at.%Ge	$1 \cdot 10^4$	$2 \cdot 10^{12}$	-58	0,43-0,45	$4 \cdot 10^{10}$
Si+2,2at.%Ge:B	$3 \cdot 10^4$	$4 \cdot 10^{14}$	-55	0,45	$2 \cdot 10^{10}$
Si+2,2at.%Ge:B	$5 \cdot 10^4$	$6 \cdot 10^{18}$	-70	0,3	$1 \cdot 10^{10}$

Fig. 1 shows, that dynamic shear modulus has been decreased weakly in a temperature interval of -196 °C - +20°C. In the vicinity of relaxation maximum shear modulus defect has been revealed. The shear modulus defect value is proportional to the relaxation process intensity. In the area of relaxation process activation of the defects reversible motion proceeds under influence of oscillation processes and temperature. This leads to weakening of interatomic bonding forces and respectively decreasing of mechanical modulus. This circumstance in this particular case stipulates revealing of shear modulus defects at the relaxation maximum temperature.

Undoped Si-Ge alloys in the initial state are characterized by current carrier's concentration of $\sim 10^{12} cm^{-3}$. Annealing at 800 °C temperature for 5 hrs causes weak decrease of current carriers (holes) concentration. Boron doped crystals are characterized by variation of holes concentration in 10^{12} - $10^{18} cm^{-3}$ interval. Annealing of boron doped crystals at 800 °C temperature for 5 hrs stipulates increase of carrier's concentration by 15%. This can be explained by increasing B content in solid state under influence of thermal annealing.

In the internal friction spectrum of Si-Ge alloys by increasing Ge content from 0,5 up to 2,2 % raising of relaxation processes intensity has been observed. In addition, maximum is expanded and shifted towards low temperatures. Respectively, tendency to decreasing of activation energy of relaxation process has been revealed.

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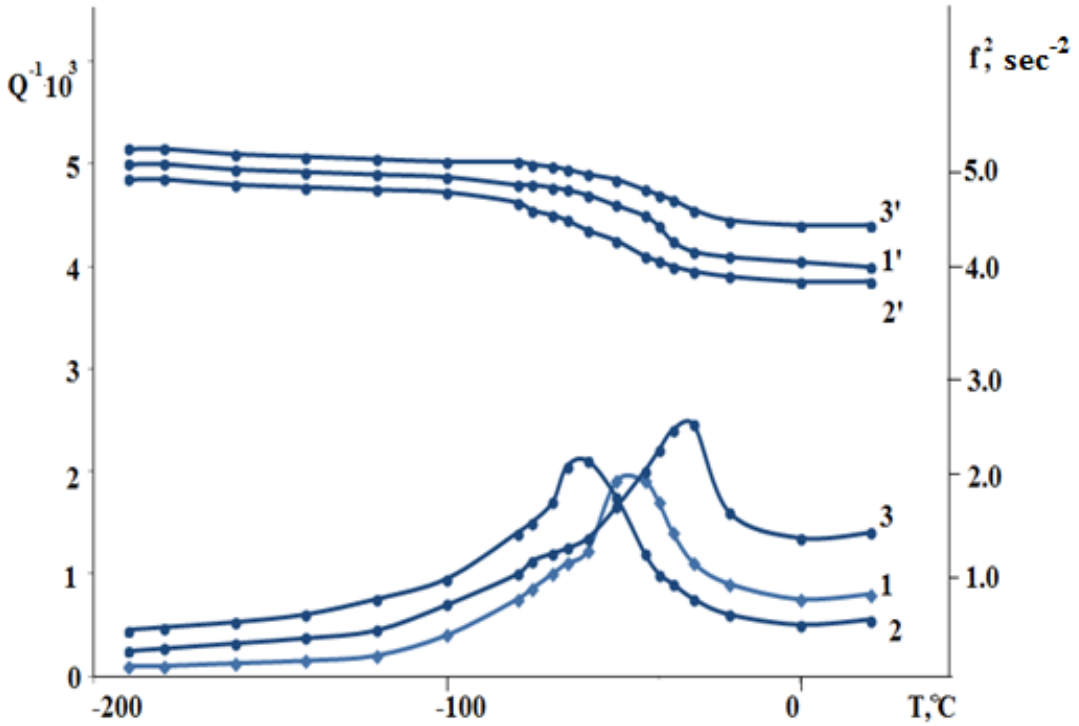

Fig.2. Monocrystalline Si-Ge alloys

internal friction (1,2,3) and shear modulus (1', 2', 3') temperature spectra

1, 1'- Si+0,5at%Ge;

2, 2'- Si+2at%Ge;

3, 3'- Si+2,2at%Ge:B ($10^{14}cm^{-3}$)

In boron weakly-doped alloys ($10^{14}cm^{-3}$) raise of internal friction background intensity has been revealed, this increase is significant in Si-Ge alloys with high Ge content. In boron doped Si-Ge alloys relaxation internal friction maximum temperature is increased by 5- 10 °C in comparison with undoped Si-Ge alloys. This circumstance indicates increasing of relaxation centers' activation energy. In low temperature interval internal friction spectrum reveals weak amplitude dependence that is enhanced at -70_ -50 °C temperatures. According to the theory [2] internal friction amplitude dependence is stipulated by dislocations and point defects' interaction. Presence of internal friction amplitude dependence at low temperatures indicates, that inelastic processes take place preferentially in the superficial layers of Si-Ge monocrystalline specimens, where generation of point defects (vacancies, impurity atoms) and high mobility dislocations is expectable.

Cyclic deformation (number of cycles -200, strain amplitude- $1 \cdot 10^{-3}$) at 800 °C temperature in vacuum causes significant increase of intensity and broadening of internal friction maximum. After hightemperature cyclic deformation internal friction maximum shifts towards the low temperatures. In the deformed state tendency to decreasing of relaxation processes activation energy has been revealed.

Annealing of cyclic deformed Si+2,2at%Ge:B($10^{14}cm^{-3}$) specimen at 800°C for 5 hrs in vacuum causes significant decrease of intensity of maximum , and also internal friction background intensity.

Structural-sensitive physical-mechanical characteristics of Si-Ge alloys doped by boron with high concentration ($10^{18}cm^{-3}$) reveal tendency to decrease. Herewith relaxation internal friction maximum shifts toward low temperatures. Relaxation process activation energy decreases. Annealing at 800 °C in vacuum for 5 hrs stipulates additional decrease of physical-mechanical characteristics unlike the identical parameters of undoped monocrystalline Si-Ge alloys.

Hightemperature cyclic deformation ($\varepsilon \approx 5 \cdot 10^{-3}$, number of cycles-500) of Si-Ge:B($10^{18} cm^{-3}$) specimens causes considerable growth (20%) of relaxation process intensity , significant decrease of its activation characteristics and weak increase of internal friction background. Subsequent annealing of deformed specimens at 600°C in vacuum for 5 hrs suppresses reduction of internal friction spectra activation characteristics.

It is known [3] that at low temperatures internal friction spectra of metallic materials are preferentially of dislocation origin. Dislocation free kinks, segments and kinks weakly pinned by point defects takes part in formation of internal friction spectra. In semiconductors at low temperatures dislocations motion is practically impossible in stress fields due to existence of high potential barrier. However, mechanical stresses in superficial structure of semiconducting crystals can stipulate various dislocations motion [4] . In the monocrystalline Si-Ge alloys superficial structure dislocations breaking from various pinning centers can be a reason for origination of relaxation type internal friction maximum and shear modulus defect revealed near to -50°C temperature. It is supposed that observed changes of relaxation processes activation characteristics are related to the variation of dislocation energetic parameters.

It is experimentally established, that intensity of lowtemperature internal friction relaxation maximum in monocrystalline Si-Ge alloys is characterized by amplitude dependence. According to the theory [5] this type relaxation processes are stipulated by dislocation kinks breakaway from the pinning defects (vacancy, impurity atom). Reduction of relaxation process activation energy, in boron heavily-doped Si-Ge crystals can be connected to weakening of dislocation blocking by pinning centers. This assumption is in agreement with the well- known theoretical models.

CONCLUSIONS

In monocrystalline Si-Ge alloys relaxation internal friction maximum and shear modulus defect have been revealed near -50°C temperature. Regularities of changing activation characteristics depending on germanium and boron concentration have been established. The investigation results of microstructure, electrophysical and mechanical properties presented in this work are significant for establishment of controlling possibilities of the physical-mechanical properties of the bulk monocrystalline Si-Ge alloys in different conditions of various origin influence. Established regularities of changing structural defects activation characteristics under influence of doping and thermal treatment are considerable for the theory of plasticity and strengthening of Si-Ge system semiconducting monocrystals.

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