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*Physics*

# Influence of Arsenic on the Physical-Mechanical Characteristics of Monocrystalline $Si_{99.97}Ge_{0.03}$:As Solid Solution

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**ABSTRACT. Physico-mechanical characteristics amplitude dependence of arsenic-doped monocrystalline $Si_{99.97}Ge_{0.03}$:As solid solution in the temperature range of 20-700$^0$C were investigated. The reasons of the variations of physical-mechanical characteristics, caused by doping, thermal treatment and high amplitude cyclic deformation, were analyzed.** *© 2010 Bull. Georg. Natl. Acad. Sci.*

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

Monocrystalline alloys of the silicon-germanium system are characterized by wide application prospects in microelectronic and optoelectronic equipments and devices. This is due to the possibilities of controlling the lattice parameters and the energy gap. For effective application of these properties, complex investigations of the process of obtaining and the fundamental physical properties of bulk monocrystalline Si-Ge alloys are important. Solution of the mentioned problems allows us to create photodetectors, X-ray and optoelectronic transducers and other electronic devices, in which Si-Ge monocrystalline alloys will be used as the substrate instead of Si.

At present, the real structure of bulk Si-Ge alloys, their mechanical and electro-physical parameters have not been complexly investigated. Practically neither have the energetic and activation characteristics of the generation of structural defects, their interactions and motions been investigated.

It is known [1-4] that variations of the concentration of Ge and dopant elements influence the formation of the dislocation structure, its mobility and physico-mechanical properties of the solid solution of the Si-Ge system.

In this paper we present the results of investigations of the amplitude dependences of the shear modulus and internal friction of n-type monocrystalline Si-Ge alloys, doped with As. Bulk monocrystalline $Si_{99.97}Ge_{0.03}$:As solid solution has been grown along the [111] direction, by the Chzochralski method. The dislocation structure on the (111) plane of the specimens was studied with the optical microscope Neophot-23. The electrophysical characteristics were established by the Hall effect. Measurements of the shear modulus and internal friction were carried out with laboratory equipment, in the range of low frequencies (0.5-5Hz). The main part of the equipment is a vertical pendulum. The test specimen is fastened to the axis of pendulum, with refractory kaolin. Under the influence of a couple of electromagnets the pendulum makes torsional oscillations.

The absolute value of the shear modulus is calculated by the method of comparing the standard and test specimens:

$$G = G_0 \frac{f^2}{f_0^2}$$

where $G_0$ and $f_0$ are the shear modulus and oscillation frequency of the standard specimen(vanadium), and $G$ and $f$ – the shear modulus and oscillation frequency of the test specimen.

The amplitude dependence of torsion oscillations at the fixed temperatures is calculated from the equation [5]:

$$\varepsilon = KTC^{\frac{1}{2}} \exp\left(\frac{H}{KT}\right)$$

where $K$ is the Boltzmann constant, $T$ – measuring temperature, $H$ – activation energy, $C$ – concentration of impurities.

The elastic limit is calculated from the equation:

$$\sigma = G \cdot \varepsilon$$

where $G$ is the shear modulus , and $\varepsilon$ – relative deformation.

The investigation involved $Si_{99.97}Ge_{0.03}$ crystals with low (~$10^{16}$ $cm^{-3}$) and high (~$10^{19}cm^{-3}$) concentration of arsenic.

On the (111) plane of $Si_{99.97}Ge_{0.03}$ :As ( $1 \cdot 10^{16}$ $cm^{-3}$) monocrystal, dislocations are irregularly distributed (Fig1,a) and their density is $1 \cdot 10^4$ $cm^{-2}$. In crystal with high ($10^4$) concentration of arsenic, dislocation groups are revealed (Fig1,b). The average value of the dislocation density is $2 \cdot 10^5$ $cm^{-2}$.

Measurements by the Hole effect show that annealing in vacuum at 700°C, for 10 hrs. causes slight increase of current carrier concentration. This is due to the increase of As concentration in the crystal by thermal treatment. This kind of thermal treatment practically does not affect the character of distribution of dislocations on the (111) crystallographic planes.

Comparative analysis of the oscillation frequencies of the standard and test specimens with identical size and shape has shown that the shear modulus of the $Si_{99.97}Ge_{0.03}$ monocrystal with high concentration of As is lower by 15% than the shear modulus of specimens with low concentration of As. Annealing in vacuum at 700°C causes an increase of the shear modulus. Being significantly manifested in Si-Ge monocrystals with low concentration of As. The physico-mechanical characteristics of the test specimens in the initial state are presented in Table 1.

On the curve of internal friction amplitude dependence of $Si_{99.97}Ge_{0.03}$ monocrystal, weakly-doped with As, superposition of three processes is observed: one at low amplitudes, in which internal friction practically remains constant with increasing vibration amplitude, the second one gives a slow linear rise at intermediate amplitudes and the third increases rapidly with amplitude at high vibration amplitudes.

The multistage character of the IF amplitude dependence confirms the variation of the mechanism of the processes of dissipation of mechanical energy in a wide range of torsion deformation amplitudes in the arsenic-doped $Si_{99.97}Ge_{0.03}$ monocrystalline solid solution.

Increase of temperature causes the decrease of critical values of vibration amplitude, which separate internal fric-

a) x200 b) x200

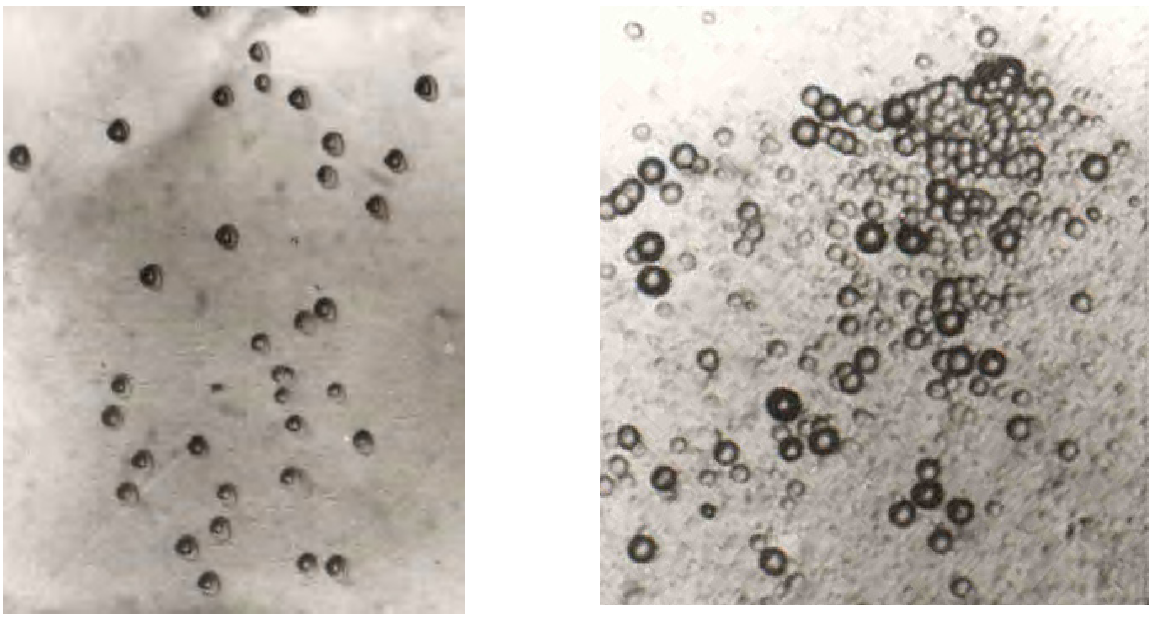

Fig.1. Microstructure of monocrystalline $Si_{99.97}Ge_{0.03}$:As solute solution a) $Si_{99.97}Ge_{0.03}$:As ($1 \cdot 10^{14}$ $cm^{-3}$) b) $Si_{99.97}Ge_{0.03}$:As ($5 \cdot 10^{19}$ $cm^{-3}$)

Table 1

Physico-mechanical characteristics of monocrystalline $Si_{99.97}Ge_{0.03}$:As

| Specimens | Temperature, $^{0}C$ | Carrier concentration, $cm^{-3}$ | Shear modulus, $kg/mm^2$ | I critical amplitude $x10^4$ | II critical amplitude $x10^4$ | I Elastic limit $kg/mm^2$ | II Elastic limit $kg/mm^2$ |
|---|---|---|---|---|---|---|---|
| $Si_{99.97}Ge_{0.03}$:As | 20 | $1{\cdot}10^{16}$ | 4700 | 0.8 | 5 | 0.38 | 2.35 |
| | 100 | – | 4600 | 0.7 | 4 | 0.32 | 1.84 |
| | 200 | – | 4530 | 0.6 | 3.5 | 0.27 | 1.58 |
| | 300 | – | 4400 | 0.5 | 3.0 | 0.22 | 1.32 |
| | 400 | – | 4350 | 0.45 | 2.5 | 0.19 | 1.08 |
| | 500 | – | 4270 | 0.4 | 2.0 | 0.18 | 0.85 |
| | 600 | – | 4160 | 0.3 | 1.5 | 0.12 | 0.62 |
| $Si_{99.97}Ge_{0.03}$:As | 20 | $5{\cdot}10^{19}$ | 4620 | 0,45 | 1 | 0,21 | 0,46 |
| | 100 | – | 4550 | 0.4 | 0.9 | 0,18 | 0,41 |
| | 200 | – | 4460 | 0.35 | 0.8 | 0,16 | 0,36 |
| | 300 | – | 4300 | 0.3 | 0.6 | 0.13 | 0.26 |
| | 400 | – | 4270 | 0.25 | 0.55 | 0.11 | 0.23 |
| | 500 | – | 4220 | 0.2 | 0.5 | 0.08 | 0.21 |
| | 600 | – | 4100 | 0.15 | 0.4 | 0.07 | 0.16 |

tion processes of different origin. Under the value of critical amplitude II variation of the internal friction is reversible. From critical amplitude II, at the return curve, internal friction of hysteretic types is revealed. In the range of high amplitudes ($\varepsilon \geq 5{\cdot}10^{-3}$) cyclic deformation at 600°C (number of cycles - 200) causes hysteretic variations of internal friction in the vicinity of room temperature, which was revealed at the return curve of IF amplitude dependence, in the range of $10^{-4}$ - $5{\cdot}10^{-3}$ amplitude deformation.

It is known [5] that occurrence of internal friction maximum of hysteretic type is a result of generation of new dislocations, at high amplitudes under the influence of deformation. Increase of the measuring temperature up to the 700°C practically does not influence the multistage character of internal friction amplitude dependence. At increased temperature, the values of critical amplitude decrease and internal friction intensity increases. Variation of the internal friction amplitude dependence has been revealed in the temperature range of 20-700°C. Increase of temperature causes the decrease of the values of critical amplitude deformation and increase of intensity of internal friction background by 15-20%. The absolute value of shear modulus linearly decreases with increasing temperature. Its value decreases by 12%, in comparison with the value measured at room temperature. Temperature decrease of the values of shear modulus and critical amplitude deformation causes a decrease of the elastic limit (Table 1).

Annealing in vacuum at 700°C, for 5 hrs. reveals the tendency to slightly increase the physico-mechanical characteristics. This is the result of the existence of strong links of dislocations with impurity atoms (especially oxygen). Thermal treatment at the intermediate temperatures (600-900°C) slightly changes the impurity concentration, in the Kottrell atmosphere and core of dislocation.

Internal friction multistage amplitude dependence is preserved in the case of high concentration of arsenic ($5{\cdot}10^{19}$ $cm^{-3}$). In this value of elastic limit, shear modulus and critical amplitudes are significantly reduced. Around the As atoms, the crystalline lattice of the Si-Ge solid solution is characterized by tensile deformation, which causes a decrease of interatomic bonding forces and respectively of the shear modulus.

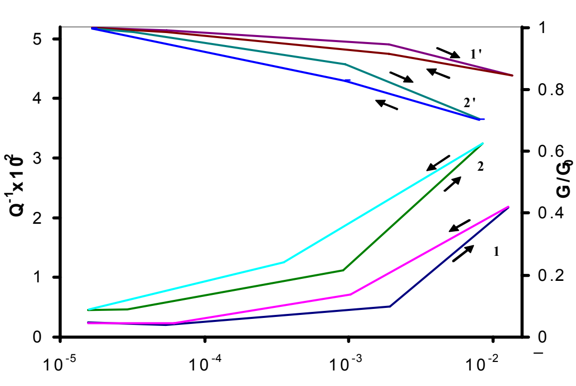


Fig. 2. Amplitude dependence internal friction (1,1') and relative shear modulus (2.2') of monocrystalline $Si_{99.97}Ge_{0.03}$:As solid solution at T=20°C

Herewith, in the conductive zone, free electrons, of high concentration decrease the interatomic bonding forces. This causes an increase of dislocation mobility and decrease of elastic limit and development of microplastic deformation. These variations are revealed on the curves of shear modulus amplitude dependences (Fig. 2, 1′) and (Fig. 2, 2′). At the critical amplitudes kinks have been revealed on the curve of shear modulus. Under the high amplitude influence, hysteretic type decrease of shear modulus has been revealed on the return curve of amplitude dependence. This is the result of the generation of new dislocations and breakaway of segments from the strong pinning centers.

Experiments show that As atoms brake dislocations and cause an increase of the mechanical characteristics in the $Si_{99.97}Ge_{0.03}$ solid solution with low concentration of arsenic. In the case of high concentration of arsenic, two processes take place – decrease of interatomic bonding forces under the influence of free electrons and breaking of dislocations with As atoms and its complexes. By doping and thermal treatment, it is feasible to control these processes and electrophysical properties, which is important in the practical use of Si-Ge monocrystals.

*ფიზიკა*

# დარიშხანის გავლენა მონოკრისტალური $Si_{99.97}Ge_{0.03}$:As მყარი ხსნარის ფიზიკურ-მექანიკურ მახასიათებლებზე

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**შესწავლილია 20-700°C ტემპერატურულ ინტერვალში დარიშხანით ლეგირებული მონოკრისტალური მყარი ხსნარის ფიზიკურ-მექანიკური მახასიათებლების ამპლიტუდური დამოკიდებულება. გაანალიზებულია ლეგირების, თერმული დამუშავებისა და მაღალამპლიტუდური ციკლური დეფორმაციით გამოწვეული ფიზიკურ-მექანიკური მახასიათებლების ცვლილების მიზეზები.**

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