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*Physical Chemistry*

# Peculiarities of the Internal Friction Spectrum of Ceramic-Metal $Si_{0.8}Ge_{0.2}$:P Alloys

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**ABSTRACT. Internal friction and shear modulus temperature dependence of ceramic-metal Si-Ge alloys doped with phosphorus were investigated. Relaxation processes occurring by the motion of defects of dislocation origin were revealed. Activation characteristics of defects motion were established.** *© 2010 Bull. Georg. Natl. Acad. Sci.*

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

Polycrystalline alloys of Si-Ge n- and p-type are characterized by wide application prospects in thermoelectrical devices, which work at high temperature 1000-1200$^0$C [1]. An effective method of obtaining bulk Si-Ge samples with ultra-granular structure is hot pressing in the 1100-1300$^0$C temperature range. Practically structural-sensitive physico-mechanical properties of such alloys have not been investigated [2].

Ceramic-metal Si-Ge alloys doped with phosphorus are characterized by n-type conductivity. In the crystalline lattice of Si-Ge alloys, near P atoms elastic deformation fields are formed. Under their influence diffusive activity of impurities is increased and energetic conditions of generation and mobility of different types of dislocations are changed. With increase of carrier concentration, disconnected electron couplings are compensated in the dislocation core, which causes an increase of dislocation mobility. In the P-doped Si-Ge crystal simultaneously acting local deformation fields, near atoms of doping elements and electron bonding forces, cause decrease of energetic barrier to the dislocation motion. Both of these factors determine the peculiarities of the internal friction temperature spectrum in P-doped Si-Ge crystals. In high temperature range of spectrum stress relaxation, localized on the interface of particles of compacted alloys, is possible. It has an influence on the activation energy and diffusive activity of components in the interfacial areas.

Internal friction and shear modulus temperature spectra of ceramic-metal samples of thermo electrical $Si_{0.8}Ge_{0.2}$:P alloys are presented in the present paper. Carrier concentration is $2{\cdot}10^{20}cm^{-3}$. Internal friction temperature spectrum at frequency of 0.8Hz and vibration amplitudes of $\sim 2{\cdot}10^{-5}$ is characterized by internal friction background, dependent on temperatures and maxima at 100, 200, 280, 500, 540 and 650$^0$C temperatures (Fig 1.1′).

In the range of 300-800$^0$C temperatures superposed maxima form a spectrum of high relative intensity, this is a result of the deformed state of the specimen. After annealing during repeated measurement maxima intensity is decreased by 15-20%. Increase of oscillation frequency up to 5.0 Hz causes a shift of maxima to high temperatures, which confirms their relaxation origin. Internal friction relaxation maxima are characterized by the values of activation energy of 0.90, 1.30, 1.45, 1.65, 1.85 and

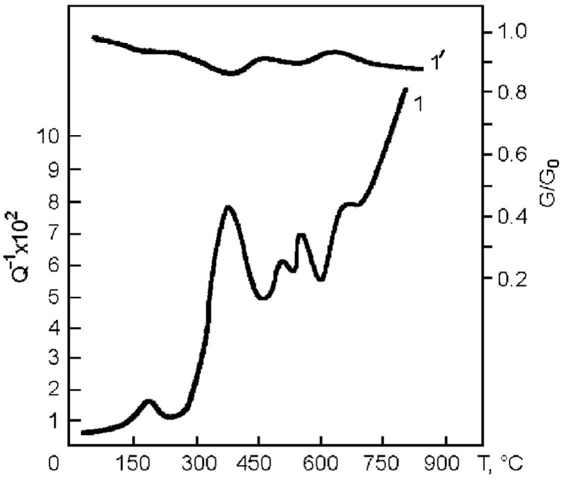


Fig. 1. Temperature dependence of internal friction (1) and shear modulus (1′) of ceramic-metal $Si_{0.8}Ge_{0.2}$:P alloys

2.60eV. Values of frequency factors are estimated from the exponential dependences of relaxation time on absolute temperature (Table 1).

On the curve of relative shear modulus temperature dependence, shear modulus defects are revealed. Their values are proportional to the intensity of internal friction maxima (Fig.1.1′). Increase of shear modulus is revealed at the 400-450, 500-600 and $700^0$C temperatures. It can be caused by phase transformation in the localized areas in the real structure of crystal. The influence of temperature and external stress causes distribution of point defects in the core of dislocations, increase of impurity concentration in the Kottrell atmosphere and dynamic strengthening of structure. Annealing in vacuum at $600^0$C, for 5 hrs. causes suppression of relaxation process at $100^0$C. Analogous maxima of undoped and B-doped Si-Ge alloys show high thermal stability [3].

An increase of critical temperatures of the rest of maxima by $10\text{-}20^0$C is revealed. The values of activation energy of defects motion are increased too, in the 300-$800^0$C temperature range. Internal friction intensity is independent of the vibration amplitude in the $5\cdot10^{-5}$-$1\cdot10^{-4}$ deformation interval, in a wide temperature range. That can be accounted for by diffusive saturation of impurity atmosphere around the dislocations and generation of oxygen metastable complexes, which cause effective fastening of dislocations.

Cyclic deformation at room temperature at $5\cdot10^{-3}$ deformation amplitude causes an increase of the internal friction background by ~20%, in the 20-$300^0$C temperature range. Relaxation maxima intensity and shear modulus defects practically do not change. After cyclic deformation at $400^0$C a sharp rise of internal friction intensity is revealed in the 300-$800^0$C temperature range. Strong amplitude dependence of internal friction background is revealed in the high temperatures range in the deformed crystal. This is connected with a decrease of the activation energy of relaxation centers migration in the cyclic deformed P-doped specimens. Decrease of activation energy of relaxation maxima of deformation origin is connected with local decrease of Pierlles potential barrier [4].

Annealing at $800^0$C, for 5 hrs. causes increase of critical temperature of internal friction background by ~$60^0$C and deformation origin maxima shift to the high temperatures by 20-$30^0$C. In the internal friction spectrum relaxation maxima are revealed at the increased temperatures in annealed specimens.

It must be noted that complexes of Ge and P-Ge have different thermal stability and deformation degree (quality), which is localized in the crystalline lattice of diamond types on the base of Si. With the ceramic-metal technology, variations of dislocation density, concentration of vacancies and doping atoms and changes of energies of interaction, motion and generation of defects are feasible. Those are revealed by the peculiarities of variations of energetic characteristics of inelastic properties, caused by thermal treatment and cyclic deformation (Table 1).

The obtained results can be used for analysis of mechanisms of electrons and phonons scattering in crystalline lattice of thermoelectrical Si-Ge alloys.

Table 1

Activation characteristics of relaxation processes of ceramic-metal $Si_{0.8}Ge_{0.2}$:P alloys

| Specimen | Max. Temperature, $^0$C | | | Activation energy, eV | | | Frequency factor, sec$^{-1}$ | | |
|---|---|---|---|---|---|---|---|---|---|
| | Initial state | Annealing $600^0$C, 5hrs. | Cyclic deformation $600^0$C, $\varepsilon=5\cdot10^{-3}$ | Initial state | Annealing $600^0$C, 5hrs. | Cyclic deformation $600^0$C, $\varepsilon=5\cdot10^{-3}$ | Initial state | Annealing $600^0$C, 5hrs. | Cyclic deformation $600^0$C, $\varepsilon=5\cdot10^{-3}$ |
| $Si_{0.8}Ge_{0.2}$:P $n=2\cdot10^{20}cm^{-3}$ | 80-100 | 80-100 | 80-100 | 0.90 | 0.90 | 0.90 | $3\cdot10^{14}$ | $3\cdot10^{14}$ | $3\cdot10^{14}$ |
| | 200 | 200 | 200 | 1.35 | 1.35 | 1.30 | $7\cdot10^{13}$ | $7\cdot10^{13}$ | $6\cdot10^{13}$ |
| | 370 | 390 | 380 | 1.40 | 1.50 | 1.35 | $3\cdot10^{12}$ | $4\cdot10^{12}$ | $1\cdot10^{12}$ |
| | 490 | 500 | 485 | 1.55 | 1.75 | 1.60 | $6\cdot10^{11}$ | $7\cdot10^{11}$ | $5\cdot10^{11}$ |
| | 525 | 640 | 620 | 1.85 | 1.95 | 1.80 | $2\cdot10^{11}$ | $3\cdot10^{11}$ | $1\cdot10^{11}$ |
| | 625 | 540 | 530 | 1.70 | 1.80 | 1.75 | $4\cdot10^{11}$ | $6\cdot10^{11}$ | $1\cdot10^{12}$ |

*ფიზიკური ქიმია*

# მეტალოკერამიკული $Si_{0.8}$-$Ge_{0.2}$:P შენადნობების შინაგანი ხახუნის სპექტრის თავისებურებანი

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**შესწავლილია ფოსფორით ლეგირებული $Si_{0.8}$-$Ge_{0.2}$ მეტალოკერამიკული შენადნობის შინაგანი ხახუნისა და ძვრის მოდულის ტემპერატურული დამოკიდებულება. გამოვლენილია დისლოკაციური წარმოშობის დეფექტების მოძრაობით გამოწვეული რელაქსაციური პროცესები და განსაზღვრულია დეფექტების მოძრაობის აქტივაციური მახასიათებლები.**

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