THERMAL EXPANSION OF POLYCRYSTALLINE $SI_{1-X}GE_X(X\leq0.02)$ ALLOYS IN THE 20-800°C TEMPERATURE INTERVAL

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Abstract

Study of polycrystalline Si-Ge alloys thermal expansion by means of dilatometric method in the wide temperature range (20-800°C) is conducted. Experiments are performed on dilatometer with quartz gauges, which is equipped with displacement capacitor sensor, featuring information exchange digital port. A special program is utilized for reading data from the sensors and processing algorithms via RS232 interface.

Experimentally is demonstrated non-monotonic changes of thermal expansion linear coefficient in a wide temperature range. A comparative analysis of temperature dependence of the thermal expansion coefficient for SiGe alloys was conducted. It is show that an increase in the concentration of the Ge results into a decrease of critical temperature of non-monotonic decline of linear thermal expansion by 20-30°C. All samples are characterized by clearly manifested non-monotonic temperature changes of thermal expansion, when the temperature changes at the rate of 3-5°C/min.

The experimental results referred above suggest that the non-monotonic thermal expansion of SiGe polycrystalline alloys in the range of 200-500°C could be caused by configuration and concentration transformations in structural defects.

Keywords: ***Silicon, Germanium, alloy, thermal expansion, structural defects***

1 Introduction

Mechanisms of defects formation in bulk crystal silicon-germanium alloy based substrates and heterostructures, their influence on the fundamental properties and their transformation under radiation and thermal treatment is insufficiently studied. This significantly hinders the use of silicon-germanium alloys in semiconductor devices.

It is known that in the diamond cubic crystal structure of silicon, defects (vacancies and their complexes, various types of dislocations, dispersed phases, impurity atoms) cause deformation in the covalent bonds and incur non-monotonic changes of material properties [1, 2, 3]. Concentration and configuration changes in the defect structure of the SiGe alloys can effectively be examined by complex research of thermal, mechanical and structurally sensitive electro-physical properties of material in a wide temperature range. It should be noted that the silicon-germanium bulk crystals thermal expansion is less studied.

2 Experimental Results

2.1 Methodology

We report the studies of polycrystalline Si-Ge alloys thermal expansion by means of dilatometric method in the wide temperature range (20-800°C). Experiments are

performed on dilatometer with quartz gauges, which is equipped with displacement capacitor sensor, featuring information exchange digital port. A special program is utilized for reading data from the sensors and processing algorithms via RS232 interface. The microstructure was investigated by the optical microscope NMM-80RF/TRF. Electrophysical characteristics were determined in the constant magnetic field of 0.5 Tesla induction on the Ecopia HMS-300 device by the Hall effect measurements.

2.2 Results and analysis

Grained structure of Germanium-doped silicon is presented on Fig.1. The boundaries of grains with relatively large size are predominantly rectilinear. The grain size of test samples range in the $5x10^{-5}$ - 10^{-3} m interval.

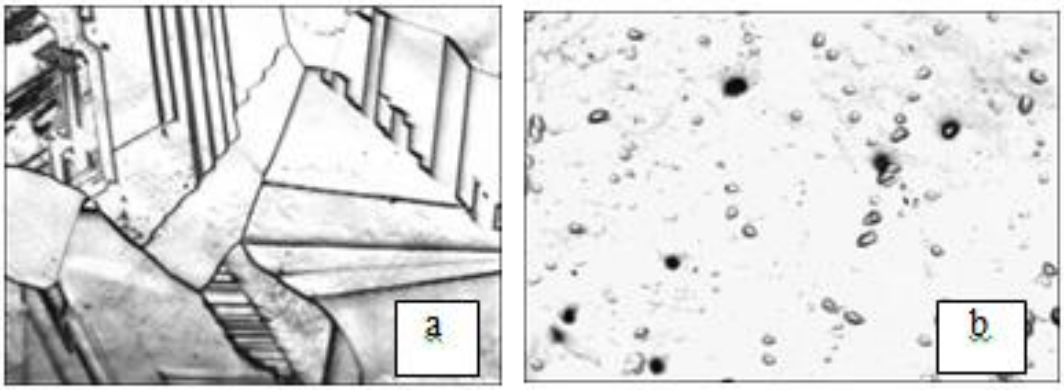

Figure 1. A microstructure of the coarse-grained Si+1at.% Ge alloy:
a - individual and grouped twins; b - an uneven dislocation distribution in the grain structure

One can observe individual and grouped twins in the sample grain structure (Fig. 1,a). Dislocation etch differ in form and size (Fig. 1,b). The change in shape is due to the crystallographic disorientation in the local areas. An increase in concentrations of germanium leads to the propagation of defects, reveals their disordered distribution, creates a new type of defects. The microstructures of undoped Si+2at.%Ge alloys feature zig-zag-type groups of stacking faults (Fig. 2)

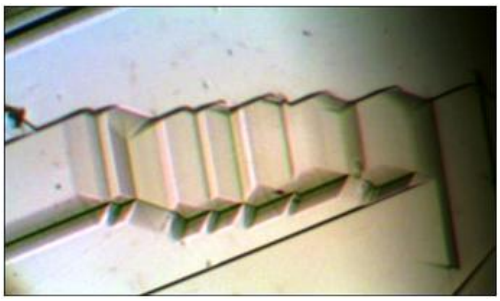

Figure 2. Microstructures of undoped Si+2at.%Ge alloys

The table presents electrophysical characteristics of polycrystalline Si-Ge alloys with various concentrations. As expected, the doping of polycrystalline silicon with the isovalent germanium impurities only slightly changes the electrophysical characteristics. All specimens are characterized by holes conductivity.

Electrophysical characteristics of polycrystalline SiGe alloys.

Table

Sample	Holes Concentration[cm-^{3}]	Mobility [cm^2/(V·s)]
Si	10^{14}	280
Si+1.5at.%Ge	$8.9x10^{14}$	170
Si+2at.%Ge	$5x10^{14}$	110

Studies of electrical conductivity σ (t) of the samples were also performed. The conductivity of the undoped coarse-grained Si and Si+2at.%Ge crystals are featuring distinct deviation from the expected linear relationship of σ(t) (See Fig. 3).

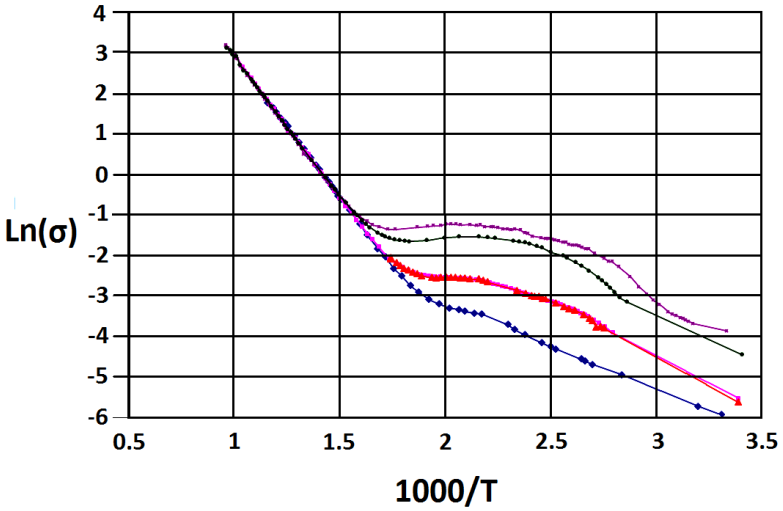

Figure 3. Temperature dependence of electrical conductivity of coarse-grained Si+2at.%Ge alloys: a-initial characterization; b-annealing 2 hours at 700°C; c-annealing 3 hours at 300°C; d-annealing 2 hours at 750°C; e-annealing 2 hours at 850°C

The above referenced results show that Si+2at.%Ge alloys demonstrate transformation of impurity conductance to self-conductance in the 180-230°C range. Slight deviations from linear change of self-conductance are observed at 450-500°C, 600°C and 680-730°C. Annealing (at 650°C) causes a decrease in the concentration of diffusion active defects distributed in the electrical active regions. This is clearly seen when samples annealing at 700°C, demonstrate reduced electrical conductivity in the 20-200°C interval.

A profound analogy of anomaly behaviour can be observed when comparing the temperature dependence of Si electrical conductance with that of SiGe. This can mainly be attributed to the nearly identical structure. A key contributor to the difference is primarily caused by relatively high concentration and random distribution of defects in Si+2at.%Ge alloys. The abnormal changes in the electrical conductivity are due to concentration of relatively small defects in the vicinity of boundaries as well as thin twins and stacking faults, dislocation and point defects.

A linear change of temperature dependence of the test specimen's relative elongation in the initial condition is characterized by deviations in the 200-260°C and 450-550°C

interval. The intermediate temperature range of 260-450°C relative elongation is non-linear. As can be seen on Fig. 4, In an event of gradual temperature reduction the relative elongation is closely matching to the results received in conditions of gradual temperature increase.

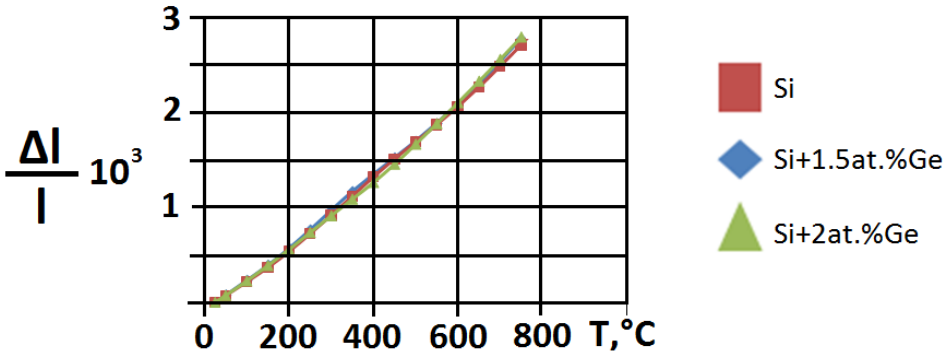

Figure 4. Temperature dependence of the relative elongation of p-Type SiGe alloys

We used experimental data of relative elongation to calculate values of linear thermal expansion α(T). As already referred on Fig. 4, thermal expansion coefficients feature deviation from linear relationship in the 200-500°C intervals. Relatively high concentrations of Ge in the alloys demonstrate zig-zag type increase of thermal expansion coefficient in the same temperature regime (see Fig. 4,5).

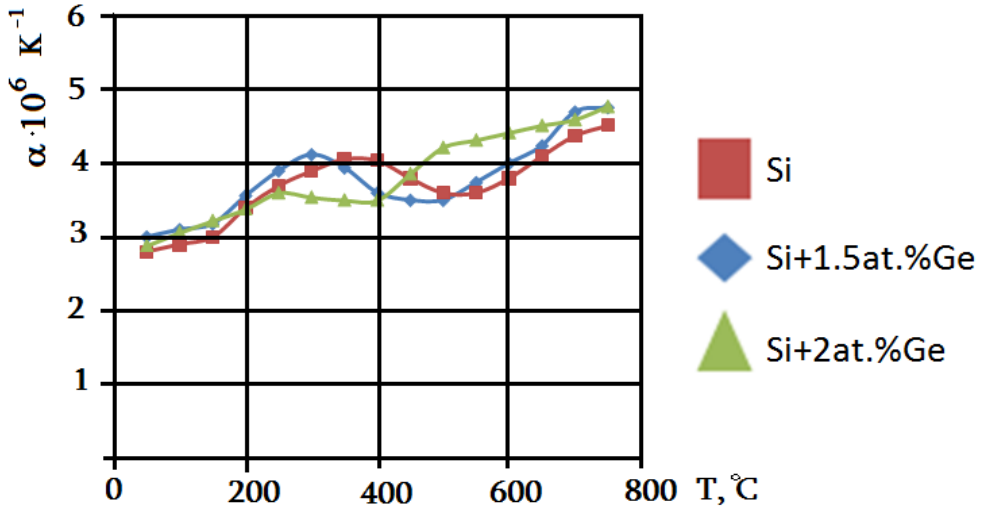

Figure 5. Temperature dependence of the thermal expansion coefficient of p-type SiGe alloys

We have seen a trend of increase of initial temperatures of the non-linear change in thermal elongation on the thermally treated samples (see fig. 6). At low temperatures (≤500°C), when annealed for 3-5 hrs, we do not see any effects on the abnormal change of relative elongation. Only the initial temperatures are indicating shift by 10-15°C towards higher temperatures.

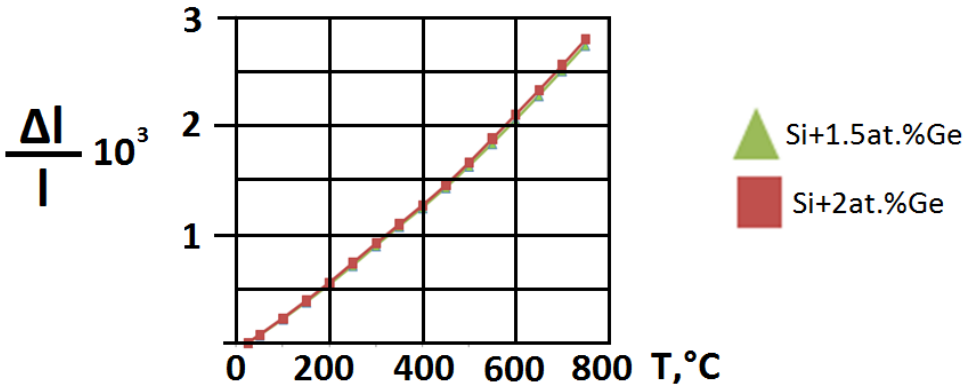

Figure 6. A temperature dependence of relative elongation of polycrystalline p-type Si+1.5at.%Ge and Si+2at.%Ge alloys after annealing at 900°C for 2hrs., V=3°C/sec

Figure 7 ghow the temperature dependence of linear expansion coefficients of SiGe alloys. It seems that the anomaly of α(T) in the samples with high Ge start on relatively low temperatures (by 20-30°C). At the same time a relatively high values of α(T) of Si+2at.%Ge are observed in the wider temperature range.

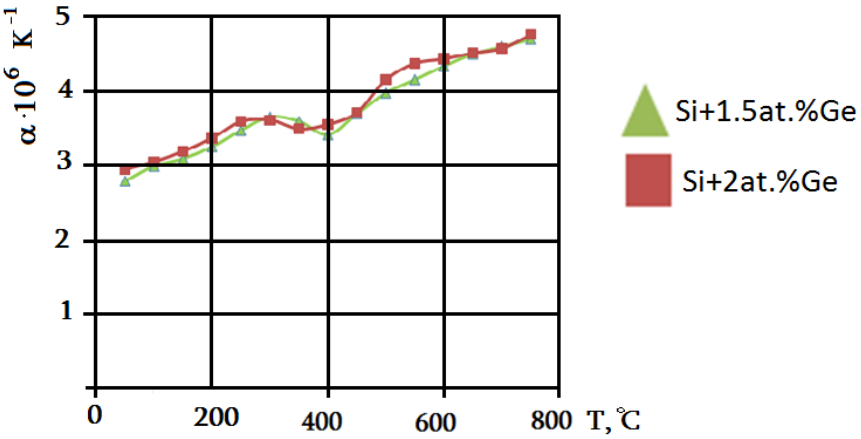

Figure 7. A temperature dependence of linear thermal expansion of polycrystalline p-type Si+1.5at.%Ge and Si+2at.%Ge alloys after annealing at 900°C for 2hrs

We have experimentally demonstrated that the polycrystalline SiGe alloys thermal expansion non-monotonic changes are clearly reveal when the temperatures are changed at the rate of 3-5°C/sec. A clear manifestation of structurally sensitive physical and mechanical properties at given rates is typical for a diffusionless phase transformations. The formation of anomalies of thermal expansion is strongly attributed to impurity atoms and dislocation origin defects. It is expected that when annealing at high temperatures, Cottrell atmospheres are formed around of dislocations. It is reported that in mono- and polycrystalline semiconductors, physical and mechanical properties in the wide temperature range are characterized by abnormal changes, what type processes is probably attributed by phase transformation in the crystal structure [4]. The structural phase transitions in high purity semiconductors are usually characterized by a minor heat

effects and small variations of lattice constant. Their spacing may vary, depending on the heterogeneity change. For example, an uneven distribution of impurities in the crystal lattice of Si results into formation of spectrum of critical transformation temperatures. Accordingly, phase transformation processes on the charts of structurally sensitive physical properties are showed the finite temperature range. Such behaviour is characterized by thermal expansion of p-type polycrystalline SiGe alloys in the 20-800°C temperature range.

3 Conclusion

It is likely that non-monotonic changes of thermal expansion are significantly attributed to impurity atoms and dislocation defects (edge and screw dislocations, stacking faults,deformation twins).

Based on the experimental results, we suggest that the non-monotonic thermal expansion of polycrystalline SiGe alloys in the 200-500°C temperature range can be caused by configuration and concentration in the transformations structural defects.

R E F E R E N C E S

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