PECULIARITIES OF "ALLOY" SCATTERING IN SEMICONDUCTORS

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The effect of nanometer size disordered regions in Si_xGe_{1-x} and InP_xAs_{1-x} semiconductor alloys on the mobility ofcharge carriers has been investigated. The investigation has shown, that the composition dependence of the mobility appears as a result of contribution of main processes of current carriers scattering on phonons, ionized impurities and "alloy" disorders in Si_xGe_{1-x} and InP_xAs_{1-x} alloys. We have calculated the contribution of these scattering processes towards total scattering. Share of contribution of "alloy" disorders into the total mobility is different for Si_xGe_{1-x} and InP_xAs_{1-x} solid solutions. Unlike Si_xGe_{1-x} alloys, the "alloy" disorders in InP_xAs_{1-x} practically do not disturb the crystal lattice in a tangible way at temperatures in the range of 4.2 – 300 K because of sublattices of InP and InAs retain certain individuality in InP_xAs_{1-x} alloys.

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Introduction

Studies of semiconductors have shown that there might be various types of heterogeneity, which have independent scientific and practical interest in terms of materials with nanometer size disordered regions. The presence of such regions may seriously alter the transport and other properties of semiconductors. These disorders are of different origin, associated with a non-uniform distribution of impurity ions in doped and compensated semiconductors,[1] arisen at irradiation[2] and at the growth of crystals,[3] related to the presence of crystalline boundaries in polycrystals.[4] Independently of semiconductor crystals growth methods there always exist these or those disordered areas, which are an accompanying appearance in semiconductor technology and cannot be ignored, because may contribute to the electrical,[5] optical[6] properties, etc. in a greater or lesser extent. All types of the heterogeneity listed above are caused by random space distribution of impurity ions and electrons and have electrostatic nature. The main peculiarity of these kinds of heterogeneity is that they modulate the semiconductors energy bands in a way, so that the optical energy gap remains invariable.

There may be another type of heterogeneity connected with random space fluctuations of the composition[7] so-called "alloy" disorders. This type of heterogeneity is one of the most interesting for semiconductor technology because semiconductor alloys (or so-called solid solutions) of elementary semiconductors or III–V compounds may extend the functionality and operational parameters of electronic devices based on them. Changes in the composition of these solutions allow monitoring of important physicochemical properties of the obtained materials, thereby are more widely used in modern semiconductor devices than their pure initial components. Many of semiconductor alloys devices offer higher performance compared to silicon devices and are competitive with GaAs-based products. Presently, experimental knowledge concerning "alloy" disorders in such materials is rudimentary with a few exceptions.

This paper is devoted mainly to review the influence of "alloy disorders" on the base of electrical properties in semiconductor alloys of elementary semiconductors and III–V compounds, Si_xGe_{1-x} and InP_xAs_{1-x}. Among the solid solutions, these systems are of great interest for engineering. In this paper, we have focused on the influence of "alloy" disorders on the mobility of charge carriers, the key parameter determining thermoelectric and microelectronic applications of semiconductors.

Experimental

The *p*-type Si_xGe_{1-x} ($0 \le x \le 1$) crystals were grown by the Czochralski technique. Experimental *n*-type samples of InP_xAs_{1-x} solid solutions were grown by the horizontal zone melting method. High degree of homogeneity of solid solutions was confirmed by several methods, among which the most important are X-ray microanalysis and application of Vegard law. Charge carriers mobility was evaluated from Hall-effect and conductivity measurements by a standard dc bridge technique. The standard deviation in the carriers' concentration was 8 – 10 % and that in the conductivity was 4 – 5%.

Results and discussion

Si_xGe_{1-x} Alloys

"Alloy" disorder scattering was observed for the first time in Si_xGe_{1-x} semiconductor alloys.[8] Our data of current carriers mobility (μ_{exp}) for Si_xGe_{1-x} solid solutions with nearly the same carriers concentration $n \sim 10^{16}$, 10^{17} and 10^{19} cm^{-3} are presented in Figure 1. Composition dependence of the charge carriers mobility of Si_xGe_{1-x} solid solutions at 300 K with the carriers concentrations $n \sim 10^{16}$ and $10^{17}cm^{-3}$ (Figure 1) reveals strong minimum in the middle of solid solutions system.

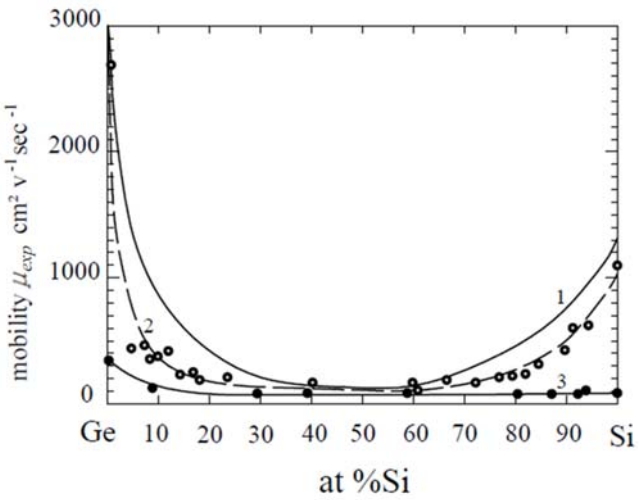

Figure 1. Composition dependence of the mobility charge carriers (μ_{exp}) at 300 K for Si_xGe_{1-x} alloys with charge concentration: 1= 1 x 10^{16} cm^{-3}, 2 = 1 x 10^{17} cm^{-3} and 3 = 2 x 10^{19} cm^{-3}.

The presence of minimum in composition dependence of mobility is defined by "alloy" scattering.[5,7] To achieve complete agreement between experimental results and the theory, it is necessary to assume the existence of an additional mechanisms of the current carriers scattering due to the disordered arrangement of solid solution atoms. Hence, we considered simultaneous action of different kinds of carriers scattering in Si_xGe_{1-x} alloys viz., the alloy disorder scattering, the scattering on acoustic lattice vibrations and the scattering on impurity ions. The individual share of contribution of these scattering mechanisms to the total varies with the compositions of Si_xGe_{1-x} solid solutions. To compare the experimental results with the theory in impurity-doped Si_xGe_{1-x} alloys, a relationship (eqn. 1), which takes into account simultaneous presence of scattering processes with different energetic dependences, was used.[9,10] The net mobility (μ) depends on the various mobility components, associated with each scattering mechanism.

$$\frac{1}{\mu} = \frac{1}{\mu_{\text{dis}}} + \frac{1}{F}\left(\frac{1}{\mu_{\text{L}}} + \frac{1}{\mu_{\text{I}}}\right) \qquad (1)$$

where,

μ_{L}, and μ_{I} are the components related to the lattice vibrations and ionized impurity scattering respectively,

μ_{dis} is the component related to disorder scattering and F is a correction factor, which takes into account the combined effect of different scattering processes.[9]

Comparison of experimental and theoretical mobility showed that component of mobility related to alloy disorders scattering follows the law predicted by theory[5,7] in Si_xGe_{1-x} alloys.

Calculation of this contribution has been made by using an expression originally derived by Brooks.[7]

$$\mu_{\text{dis}} = \frac{(2\pi)^{1/2} e\hbar^4 N_0}{3(m^*)^{5/2}(kT)^{1/2} c(1-c)(E_{\text{a}} - E_{\text{b}})^2} \qquad (2)$$

where

N_0 is the number of atoms per unit volume,

c is the composition of one of the component of alloy,

E_{a} and E_{b} are energy-positions of edges of bands for two components of alloy.

According to Brooks[7] in alloy with disorders regions the composition changes from one region to other one at the expense of statistical fluctuations. This causes energy bands deformation, peaks and dips at the edge of bands, which looks like deformation potential in theory of scattering by thermal vibration of lattice atoms. So "alloy" scattering can be considered as "frozen" scattering by thermal vibration of lattice.[5] At low level of carriers concentration "alloy'' scattering contribution to the mobility increases with increase of alloy components content. At high level of carriers concentration the mobility does not depend on alloy components content and scattering is defined by ionized impurities (Figure 1).[10]

The "alloy" scattering of current carriers is very important for creating of effective thermoelements on the base of Si_xGe_{1-x}. The perfect combination of properties connected with "alloy" disorders and thermoelectric properties in Si_xGe_{1-x} alloys makes them high effective thermoelectric materials for use at high temperatures.[10]

InP_xAs_{1-x} alloys

Contribution of disorder scattering to the electrons mobility has been revealed also for a number of III-V compound alloys, particularly for InP_xAs_{1-x} solid solutions. Mobility data of current carriers for InP_xAs_{1-x} solid solutions with nearly the same carriers concentration $n \sim 10^{16}$ and 10^{18} cm^{-3} are presented in Figure 2.

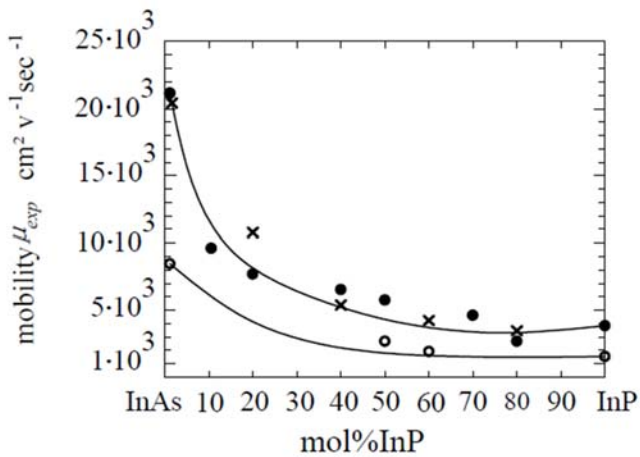

Figure 2. Composition dependence of the mobility of charge carriers (μ_{exp}) at 300 K for InP_xAs_{1-x} alloys with charge concentration = 10^{16} cm^{-3} (• – our data, × – data from ref. 11) and 10^{18} cm^{-3} (○– our data).

Composition dependence of electrons mobility at 300 K for InP_xAs_{1-x} solid solutions with the carriers concentrations $n \sim 10^{16}$ and 10^{18} cm^{-3} (Figure 2) reveals weak minimum on the InP-rich side of solid solutions system. Such character of composition dependence of mobility is connected with the change of contribution of scattering mechanisms of separate components into the total scattering at the alteration of composition. We carried out appropriate analysis of the mobility on the basis of reasonable theories.[7,9,12,13] Comparison with theoretical predictions in InP_xAs_{1-x} solid solutions with $n \sim 10^{16}$ cm^{-3} has shown that at temperatures near 300 K the prevailing mechanism is the scattering on optical phonons.[14] Contribution of the disorder scattering increases with increasing of InP composition in solid solutions system at fixed temperatures and weakens with lowering of temperature in the range of 4.2-300 K and never dominates.[15] Assumption of the existence of an additional mechanism of the current carriers scattering due to the disordered arrangement of solid solution atoms allows achieving the full agreement of experimental mobility with the theory.

The composition dependence of the mobility of current carriers for InP_xAs_{1-x} alloys (Figure 2) differs from the similar dependence for Si_xGe_{1-x} alloys (Figure 1) with well-defined minimum in the middle of alloys system. The data for alloy scattering in InP_xAs_{1-x} solid solutions do not reveal such tendency.

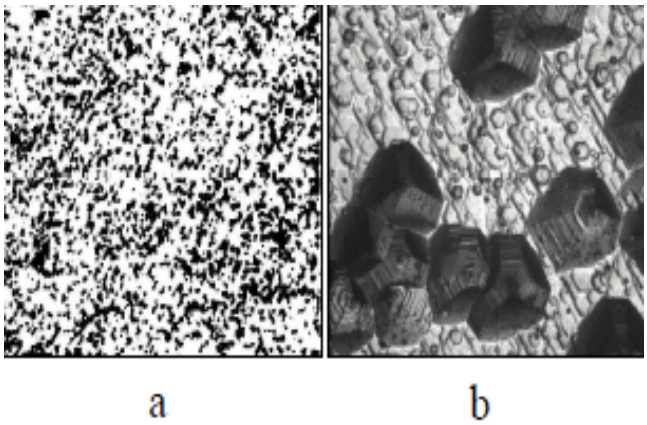

Figure 3. Dislocation structure of single crystals of semiconductor alloys on the plane (111) (a) Si_xGe_{1-x} (× 1000) and (b) InP_xAs_{1-x} (× 250).

An estimate of maximal share of disorder scattering in InP_xAs_{1-x} solid solutions results in the value which does not exceed ~ 20 % of total magnitude of determinative scattering at 300 K and ~ 10 % at lower temperatures. The reason of absence of clear minimum in the composition dependence of mobility for InP_xAs_{1-x} solid solutions may be apparently connected with the specific properties of InP_xAs_{1-x} caused by fact, that sublattices of InP and InAs retain a certain natural properties in contrast to Si and Ge in Si_xGe_{1-x} alloys. The preservation of individuality of sublattices of InP and InAs in their alloys has been previously found by us at optical properties research,[14] where has been discovered two mode behavior of lattice vibrations in InP_xAs_{1-x} alloys.

The retention of individuality of sublattices of InP and InAs in InP_xAs_{1-x} alloys is confirmed by microstructural studies (see Figure 3).

This image clearly show, that InP and InAs sublattices in InP_xAs_{1-x} alloys retain their identity as distinct from Si_xGe_{1-x} where Si and Ge do not preserve their identity.

Conclusion

Unlike Si_xGe_{1-x}, the "alloy" scattering in InP_xAs_{1-x} never dominates. In contrast to Si_xGe_{1-x}, solid solutions InP and InAs retain a certain individuality in InP_xAs_{1-x} alloys. This result means, that mobility in InP_xAs_{1-x} solid solutions is mainly defined by the factors determining III–V compounds. A relative small contribution of disorder scattering is important for devices designed on the base of InP_xAs_{1-x} system.

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