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Thermoelectric Effect in the Graded Band Gap $Si_{1-x}Ge_x$ ($0.2 \le x \le 1$), $Si_{1-x}Ge_x$ ($0.5 \le x \le 1$) Solid Solutions Dependent on the Gap Difference

A. Yu. Leiderman*, A. S. Saidov, and A. B. Karshiev

Physicotechnical Institute, Academy of Sciences of the Republic of Uzbekistan, Tashkent, Uzbekistan

**e-mail: amin@uzsci.net*

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Abstract—The thermoelectric effect, i.e., appearance of thermally stimulated current and voltage during uniform heating in a temperature range from 30 to 250°C, is studied. It is shown that greatest values of the current and voltage appear when maximum band gap difference is observed.

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Several reports on observation of the current and voltage appearing during the uniform heating of various homogeneous materials were published in the last decade. The range of these materials is very wide, from almost dielectrics, such as samarium monosulfide [1] and zinc oxide [2], to typical $A^{III}B^{V}$ semiconductors [3, 4] and polycrystalline silicon obtained by multiple remelting of technical silicon of KR-3 brand in air in a solar oven. Most recently, a similar effect was observed for the first time during the uniform heating of $Si_{1-x}Ge_x$ ($0 \le x \le 1$) solid solution film grown on a silicon substrate [6, 7]. In this case, two simple ohmic contacts were deposited on the surface of the film to observe the effect. The generated current (J) and voltage (V) reached its maximum values at a temperature of 200°C: $J \sim 3.5$ nA, $V \sim 0.3$ mV. This article is a continuation of those works and its goal is to investigate the effect of the appearance of voltage and current during the uniform heating of the $Si_{1-x}Ge_x$ ($0 \le x \le 1$) film more in detail, depending on the specific film composition.

The graded band gap $Si_{1-x}Ge_x$ ($0 \le x \le 1$) solid solution was grown by liquid phase epitaxy from a limited volume of Sn–Si–Ge solution on n-type silicon substrate with (111) orientation in the temperature range of 1000–750°C, as also described in [6, 7]. From the obtained n-type monocrystalline material, samples with length of 8 mm and thickness of 5 mm were prepared. Then, the oblique grinding of the obtained film was carried out, which made it possible to access a material with different content of germanium, with use of ohmic contacts made from silver (Fig. 1). Small resistance values of the ohmic contacts were verified by current–voltage characteristics (CVC) shown in Figs. 2a and 2b.

After that, the uniform heating of the investigated structure was conducted with a different combination of contacts: 1–3 or 1–2. The resulting thermally stimulated current and voltage are shown in Figs. 2a and 2b and also in Figs. 3a and 3b. From Figs. 2 and 3, it can be seen that the values of the current and voltage generated during the heating strongly depend on the position of the contacts and, consequently, on the composition of the film. These results and the results reported previously in [6, 7] are presented in the table.

From the results presented in table, it follows that the larger the band gap difference, the greater the observed effect: the current increases nearly fivefold, and the voltage increases by more than one order at

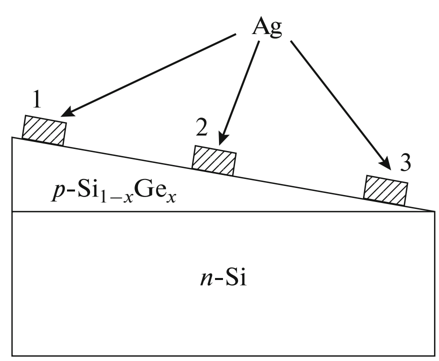


Fig. 1. Scheme of investigated p-$Si_{1-x}Ge_x$ ($0 \le x \le 1$). 1, 2, 3 are the ohmic contacts made from silver; (1) corresponds to almost 100% Ge; (2) corresponds to 55% Ge; (3) corresponds to 20% Ge.

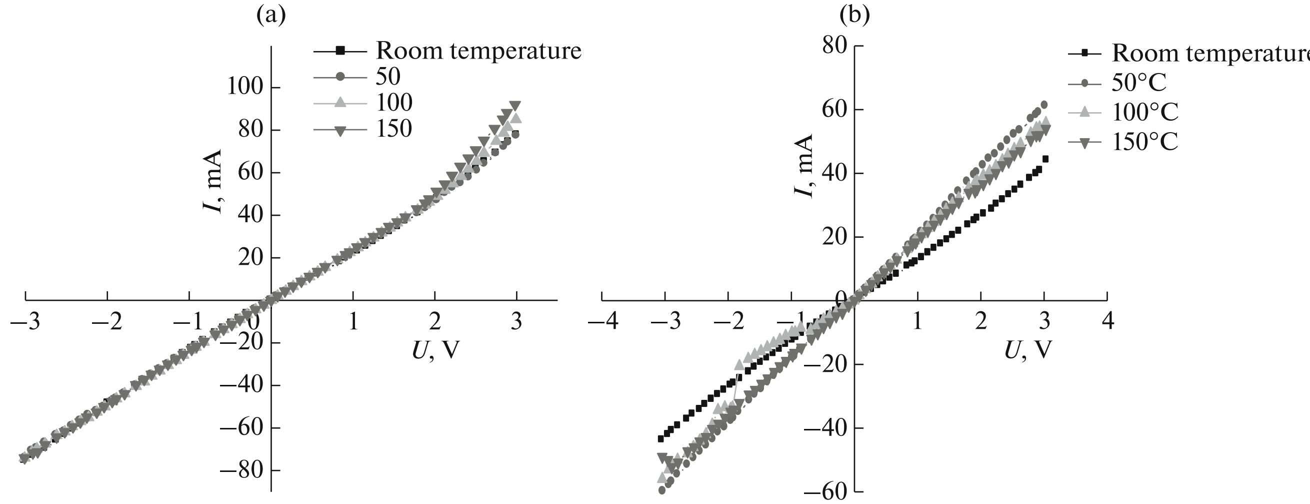


Fig. 2. Temperature dependent current–voltage characteristics of the graded band gap p-$Si_{1-x}Ge_x$ ($0 \le x \le 1$) film for different combination of the contacts: (a) 1–2 type and (b) 1–3 type.

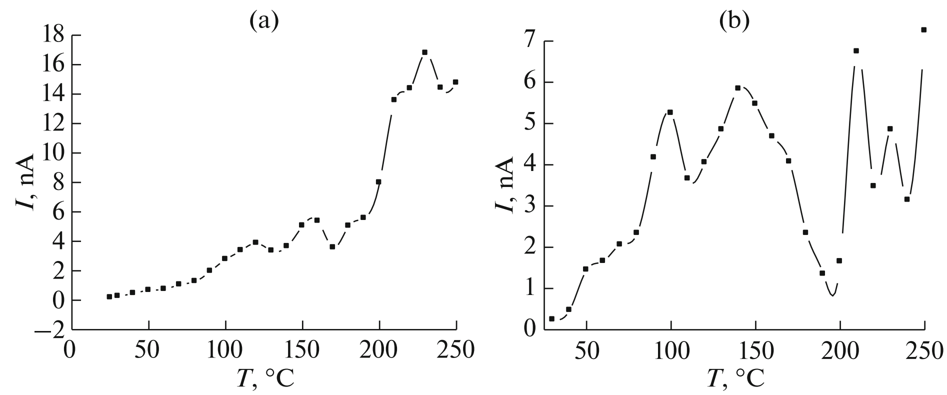
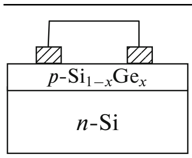
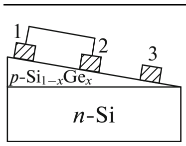
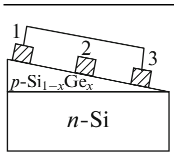


Fig. 3. Temperature dependences of currents appearing in the graded band gap p-$Si_{1-x}Ge_x$ ($0 \le x \le 1$) film for different combination of simple ohmic contacts: (a) 1–3 type and (b) 1–2 type.

Maximum values of the current and voltage generated at $T \sim 250°C$ for different positions of the contacts

Type of the contact	J_{max}	V_{max}
	3.0 nA	0.35 mV
	6.5 nA	0.65 mV
	16 nA	1.6 mV

maximum band gap difference. Of course, it is not possible to give a complete theoretical basis of the observed physical phenomena of the new thermoelectric effect immediately, but some fairly obvious considerations can be expressed. A large band gap difference is observed in the investigated solid solution, as the film composition changes through the sample thickness, from Si (1.1 eV) to Ge (0.7 eV). For the studied types of contacts, the range is slightly narrower, but still fairly large; it is approximately from 0.7 to 0.9 eV for the 1–3 contact type and from 0.7 to 0.8 eV for the 1–2 contact type. It is obvious that initial equilibrium carrier concentrations in the film are uneven; they vary with the thickness.

Therefore, it could be expected that, even after insignificant uniform heating, the carrier concentration in different positions of the film would be different, and the larger the difference in the band gap, the larger the difference in the carrier concentration would be. Obviously, in such a case, the Dember electromotive force should occur, which is described as

$$V = \frac{kT}{q}\frac{b-1}{b+1}\ln\frac{p(d)}{p(0)} \quad (1)$$

where b is the ratio of electron and hole mobilities, and $p(d)$ and $p(0)$ are the carrier concentrations on the borders of the sample, i.e., $p(0)$ is the concentration on contact 1, and $p(d)$ is the concentration on contact 2 or contact 3 depending on the conditions of the experiment. The larger the concentration difference between the values of $p(0)$ and $p(d)$, the greater the generated voltage. It is evident that the case of the 1–3 type contact corresponds to the largest difference between the $p(0)$ and $p(d)$ concentrations, as also follows from the table data.

Thus, our investigations show that the current and voltage are generated in the p-$Si_{1-x}Ge_x$ ($0 \le x \le 1$) film with simple ohmic contacts during the uniform heating, and their values are greater with a larger band gap difference in the film.

Such films, apparently, could be used for photovoltaic conversion of solar energy, since, with correctly tuned sunlight impact on them, the investigated thermoelectric effect could enhance the sunlight effect.

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