TEMPERATURE DEPENDENCE OF PHASE TRANSFORMATION PRESSURE IN SILICON[*]

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Abstract – In this experimental work the pressure induced phase transformation of silicon and Germanium has been studied. It was shown that at a particular value of applied pressure, (P_t), depending on the sample temperature, the electrical resistance of the specimen falls off to a metallic state. The main goal of this study was to find out how the phase transformation pressure, P_t, for a p-type silicon varies with the sample temperature. The results show that, the value of P_t decreases linearly as the temperature of the sample increases. Meanwhile, other related results including the rate of resistance change in accordance with applied pressure on the sample at different temperatures (~270-350K), both for the semiconductor and the metallic state of the specimen were determined. In another effort, the amount of P_t for an n-type germanium, but only at room temperature, was also determined.

Keywords – Phase transformation pressure, silicon, Germanium, metallic state, temperature dependence

1. INTRODUCTION

The results of many works show that, high tensions (Gpas.) can give rise to change in physical properties of solid materials [1-7]. One of the best examples for this phenomenon is known as the phase transformation of silicon, where the electrical resistivity of this semiconductor material in a given temperature decreases slowly with increasing the applied pressure. This procedure is continued until a critical amount of pressure is applied. There the electrical resistance of the sample falls down sharply into a semi-metallic conduction region, and its conductivity becomes comparable with a relatively poor conducting material. This evidence was initially reported by Drickamer [1]. It was believed that this sudden fall and enormous resistivity decrease of the sample is due to its phase transformation under that particular applied pressure. The results of X-ray and other analytical methods show that in the case of silicon, its metallic phase is likely to be as the β phase of Sn metal [6], where Silicon normally has a cubic diamond structure and that of β-Sn is an Orthorhombic one. Nevertheless, several theoretical and experimental results show that, under the influence of a rising pressure, Silicon undergoes various phase transformations, where each phase is defined by its own physical properties [8-10]. One of the detailed reports on the phase transformation of silicon, which was studied by XRD methods, was given by Spain [10]. In another work the pressure-induced amorphization of crystalline silicon and vice-versa have been studied [9]. According to Gib's equation in a steady state condition: P+F=C+2, where P is the number of stable phase, C the number of elementary compositions in the material concerned, F is degree of freedom and 2 is number of two physical variables, i.e., temperature and pressure, so considering the phase diagram of a particular element in terms of pressure versus temperature, different phases in various pressures for such elements are anticipated; It has been shown that in the case of pure silicon, there are

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more than ten different distinct phases in a variety of conditions [11-14]. One of the most interesting cases mentioned is the transformation of this semiconductor to a metallic phase at a particular pressure, P_t. The main goal of this study was to find out how this transformation pressure (P_t) for a p-type silicon varies with the sample temperature. Nevertheless, due to very close similarity between the crystalline structure of Si and Ge, another similar effort, the amount of phase transformation pressure of an n-type germanium have been determined at room temperature as well.

2. EXPERIMENTAL

The investigated p-type silicon samples were prepared by cutting a wafer into pieces the size of 8x3x0.5 mm. using an Isomet cutting machine. After cleaning and surface polishing in conventional procedures, two electrical contacts were made to both sides of samples using a paste of active carbon powder and adhesive mixture. While the back face of the samples were in a good condition for ohmic and thermal contact with a thick hollow sample holder made of brass. The experimental set up was in a manner that the temperature of the sample could be maintained by means of a temperature- controlled water flow through the sample holder. Figure.1 illustrates the schematic of the experimental set up. The required pressures on the sample were provided by a cone shaped indenter which was in contact with the surface of the sample. Meanwhile, a number of pre-weighted lead blocks which were put on the back plate of the indenter rod, provided the required applied loads on the sample. Having the values of these applied forces and the cross-section of the indenter tip, the relevant pressure on the sample has been determined. The experiment proceeds by measuring the electrical resistance through the compressed region of the specimen (between the indenter tip and back face of the sample). Every evaluation of resistance was carried out in accordance with any applied pressure on the sample, and the procedures proceeded for different temperatures of samples, which in turn were adjusted by the temperature of the water flowing through the sample holder. A similar experiment was also carried out for the case of an n-type germanium single crystal, but only at room temperature (~27˚C) and the amount of Pt for this sample was determined.
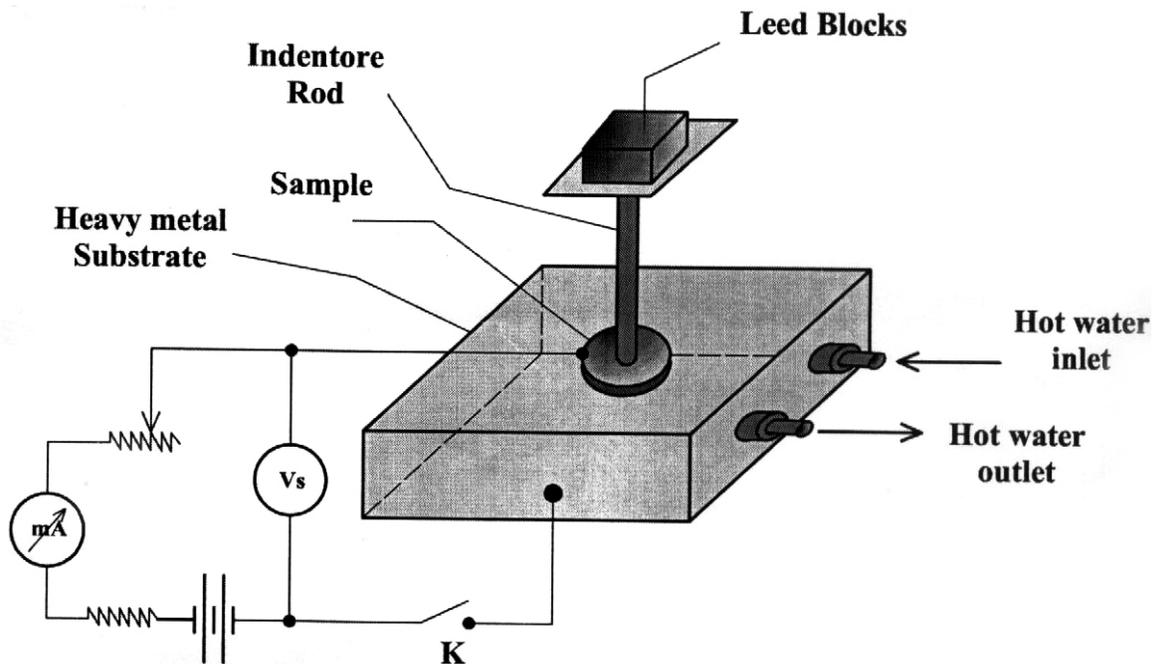

Fig. 1. Experimental set up for investigation of pressure
induced Phase Transformation in a p-type silicon

3. RESULTS AND DISCUSSION

Part of the experimental results taken at different sample temperatures of Si is illustrated in Fig. 2. and Fig. 3 illustrates the resistance change of Ge with respect to the induced pressure on the sample at room temperature. In a general view, as it is seen, there are three distinct regions on each curve of Fig. 2 and 3. In the first region, where the pressure is not sufficient for transformation to a metallic phase, the electrical resistance R of the samples varies smoothly with pressure p at a given temperature, so that the rate of dR/dp for a particular temperature seems to be constant, but R decreases linearly with increasing the applied pressure. This region can be treated as an occurrence of a slow strain within the sample which is normally anticipated for a semiconductor material, even under an elevated stress, where sufficient stress on the lattice structure will cause narrowing of the energy gap between the conduction band and valance band [4]. Since there is an exponential relation between the resistivity and energy of forbidden gap (E_g) in semiconductors, using the value of dR/dp for a given temperature from Fig. 2 or 3, and by means of some mathematical rearrangements, the rate of dE_g/dp should be estimated for a given specimen at defined physical conditions. Now, considering the second region in one of the curves in Fig. 2.which was started at a certain pressure (P_t), the resistance of the sample falls down very sharply towards a plateau region, analogous to a metallic state, meaning that the specimen has experienced a phase transformation towards a metallic state. Finally, in the third region of the graphs in Figs. (2 and 3), ie. in a semi-metallic plateau region, the rate of resistance variation with pressure is almost negligible, but is still negative as was expected. Fig 4, which was traced from the fulcrums of Fig. 2, shows a linear relation between the phase transformation pressure (P_t) and the sample temperature within the range of $250°$k to ~$350°$k. It is very clear that the value of P_t decreases as the temperature of the silicon sample increases, namely the temperature of the sample could enhance the phase transformation process in the semiconductor materials. Hence from Fig. 4, the variation rate of P_t. vs. Temperature, namely dP_t/dT was calculated to be~.041(GPs/Kelvin). Although this experimental figure does not match the previous theoretical results, the linear shape variation of P_t against temperature has been reported and confirmed by some theoretical works [15, 16]. We think that all the theoretical calculations in the frame of various models are based on the assumption of complete changes of the loaded sample to a relevant metallic state, In this case a pure metallic phase shows less response to the applied pressure than a semi-metallic case, which was practically accessible in this work. Nevertheless there is still another notable result which can be deduced from the first region of the graphs, namely the semiconductor region where for the case of the Si sample, the mean value of dR/dp was calculated for our working temperatures to be ~0.464 (Kohm/Gpas.), such a Figure. for the case of germanium, from Fig.3 became ~0.171. On the other hand, considering the amounts of Pt =8.4Gps for Si and 5.7Gps for Ge which are deduced from Figs. 2 and 3 at room temperature, and values of Eg for bough samples (1.12, 0.67ev), there is a meaningful relation between the rate of Pt(si)/Pt(Ge)=1.47 and the rate of Eg(si)/Eg(Ge)=1.67. A little discrepancy between these two Figures might be due to many other dis-similarities in the micro structural features of the two samples. Taking this fact into account, it may be deduced that there might be a linear relation between values of Pt and Eg., namely for semiconductors of similar structures. For those materials with a greater energy gap, a higher amount of Pt is anticipated.
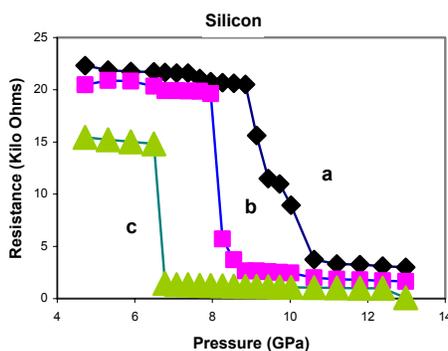

Fig. 2. Variation of electric resistance of P-type silicon Vs. pressure
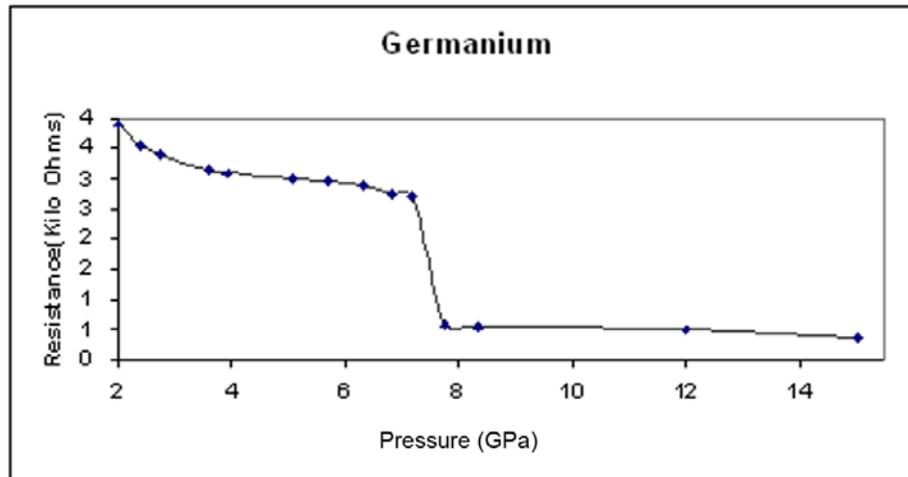at different sample temperatures: a)-5 ^{0}C ,b)20 ^{0}C, c)60 ^{0}C

Fig. 3. Variation of electric resistance of germanium
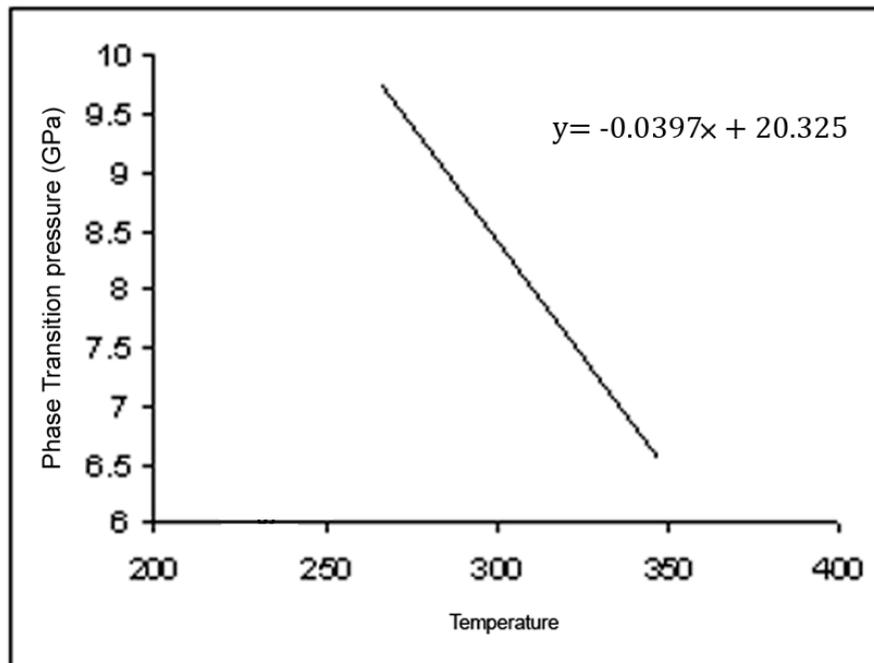N-type Vs. pressure at room temperature

Fig. 4. Variation of phase transformation pressure (Pt)
with temperature in P-type silicon

4. CONCLUSIONS

In this experimental study it has been shown that, under the applied stress the resistivity of silicon and germanium decreases linearly with increasing pressure, but at a particular value of the applied pressure P_t, and for a given temperature, resistivity falls off sharply to a metallic state, This phenomena might be interpreted as a phase transformation process of this semiconductor to a conductor state. In the case of Si it was also shown that there is an almost linear relation between the values of P_t and the sample temperatures in the range of 250K°-350K°, so that P_t decreases by increasing the temperature. Comparing the amounts of Pt for Si and Ge which have similar microstructures, shows that there is a linear relation between Pt and Eg, ie, for a bigger energy gap (Eg) a higher value of phase conversion pressure is expected.

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