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Electrical resistivity/ resistance of some semiconductors

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ABSTRACT

The resistance to flow of electrons in these amorphous semiconductors which have very high density of localized states may be controlled by hopping processes according to Lazarus. However, no theoretical calculations for the electrical resistance of these amorphous semiconductors have been carried out to the best of our knowledge. In the present work, we have tested an alternative approach which is based on the fundamental assumptions of Drickamer. It has been stated by Drickamer that the basic effects of pressure on a material are; (1) to decrease interatomic distance and (2) to increase overlap between adjacent electronic orbitals. Apart from these assumptions, Drickamer, however, has not put forward any formulation for the explanation of his measurements. A simple phenomenological formulation based on these fundamental assumptions has been tested successfully in case of some semiconductors as hydrogenated and non-hydrogenated amorphous silicon (a-Si: H and a-Si), germanium and selenium.

Key Words: a-Si: H, a-Si, Electrical resistivity, Resistance

INTRODUCTION

In recent years, considerable attention has been centered on the study of pressure dependence of electrical properties of a solid [1-3]. Such studies are of primary importance for characterization of a material and are also useful for studying the electrical transport mechanisms, details of band structure etc. While the basic factors affecting the charge conduction at high pressure are governed by some fundamental physical processes, the actual contribution to any specific electronic property may depend on the nature of the solid. For amorphous semiconductors this mechanism of electrical transport has been not yet fully understood.

According to Lazarus [4], the resistance to flow of electrons in these amorphous semiconductors which have very high density of localized states may be controlled by hopping processes. However, no theoretical calculations for the electrical resistance of these amorphous semiconductors have been carried out to the best of our knowledge. In the present work, we have tested an alternative approach which is based on the fundamental assumptions of Drickamer [5]. It has been stated by Drickamer that the basic effects of pressure on a material are; (1) to decrease interatomic distance and (2) to increase overlap between adjacent electronic orbitals. Apart from these assumptions, Drickamer, however, has not put forward any formulation for the explanation of his measurements. A simple phenomenological formulation based on these fundamental assumptions has been already tested successfully in case of materials such as polymers, semiconductors etc.

2 Formula Used for Calculations

The calculations in the present work are based on the following formula [6].

$$R(P) = A(P/Pc)^{\alpha}e^{-\beta}(P/Pc)$$

(1)

where R(P) denotes the resistance of a given solid at pressure P. A, α and β are adjustable parameters and Pc is an arbitrary pressure for making β dimensionless. Equation (1) may also be written in the logarithmic form as given below:

$$\log R(P) = \log A + \alpha \log(P/Pc) - \beta(P/Pc)$$
⁽²⁾

Since the influence of compression on the dimensions of the solid is small, one can write a similar equation for resistivity ρ in a form similar to Equation (1) as

$$\rho = A_0 (P/Pc)^{\alpha} e^{-\beta} (P/Pc)$$
(3)

$$\log \rho = \log A_0 + \alpha \log(P/Pc) - \beta(P/Pc)$$
(4)

For the sake of the comparison, the pressure coefficient of logarithm of resistivity has been also calculated here. This coefficient may be calculated from the equation (4) is written as

$$\frac{d\log\rho}{dP} = \frac{\alpha}{P} - \frac{\beta}{Pc}$$
(5)

In this paper, the resistance/resistivity calculations have been made for a number of materials. For each of the materials, the analysis has been carried out with the help of the Equations (1-4) and the results are compared with the available experimental data. The deviations between theory and experiment have been estimated with the help of a quantity:

$$S = \sum_{i=1}^{n} [\{\text{Experimental value}\}_{i} - \{\text{Theoretical value}\}_{i}]^{2}$$
(6)

Depending on the nature of the data available, the experimental or theoretical value in Equation (6) will correspond to either resistance or resistivity or some other related physical quantity. In the above equation n stands for the number of total pressures considered in the calculations. The parameters A, α and β are varied in such a manner so as to make S minimum. This ensures a best possible agreement between the theory and the experiment.

RESULTS AND DISCUSSION

According to this formulation, the resistance to the flow of electrons in a solid at high pressure may be determined by the following relation.

$$\frac{R_{\rm P}}{R_0} = A(\frac{P}{P_{\rm C}})^{\alpha} \exp\left(-\beta \frac{P}{P_{\rm C}}\right)$$
(7)

Here R_0 and R_p are the resistances of a semiconductor at ambient and high pressure P, respectively A, α and β are the parameters having values depending on the nature of the semiconductor, P_c is an arbitrary pressure introduced to make β dimensionless. The details of this formulation are underlined in Reference [6]. However, for the sake of completeness; we wish to mention some of its features in the present work also. The resistance R_p of a semiconductor may be written in the form of a following polynomial of pressure P [7].

$$R_{P} = a_{0}P + a_{1}P^{2} + a_{2}P^{3} + \cdots$$

$$R_{P} = a_{0}P(1 + b_{1}P + b_{2}P^{2} + \cdots)$$
(8)

where $b_j = a_j / a_0$ with j = 1, 2, 3...

When pressure is applied on semiconductor, it results in the overlap of charge distribution of two nearest atoms/molecules which will make a repulsive contribution to the interaction energy of two atoms/molecules. Several empirical forms describing this repulsive interaction are available in literature. According to M.P. Tosi [8], the repulsive interaction between two atoms may have the exponential form $e^{-d/B}$ where d is intermolecular co-ordinate and B is the measure of the range of the interaction. At high pressure, d will be function of P. In view of this, the quantity in bracket has been approximated by an exponential term $e^{-\beta P}$. On account of this, the equation (8) is unbalanced and this imbalance has been somewhat adjusted by putting a power of α on P. The resulting equation (7), thus, incorporates both the assumptions of Drickamer in phenomenological manner and is found to give a reasonable description of pressure induced resistance of a semiconductor.

3.1 Amorphous Silicon

Effects of hydrostatic pressure on electrical resistively of hydrogenated and non-hydrogenated amorphous silicon (a-Si: H and a-Si, respectively) at room temperature have been experimentally investigated by Lazarus [4]. From these results, one can easily extract information about the variation in electrical resistance of these semiconductors against pressure by using the value of linear compressibility ($\beta \sim 3 \times 10^{-4}$ kbar).



Fig. 1- Variation of electrical resistance of non hydrogenated amorphous silicon



Fig. 2- Variation of electrical resistance of hydrogenated amorphous silicon

The theoretical calculation for pressure dependence of electrical resistance has been carried out by changing the value of the parameters A, α and β appearing in equation (7) in such a manner so as to obtain a least square fit with the measured data. The calculated results for the two semiconductors i.e. a-Si and a-Si: H has been compared with the derived experimental data in Figure-1 and 2 respectively.

It is clear that equation (7) yields a good description of variation of electrical resistance with pressure. The values of the parameters used in the calculations are quoted in Tables 1 and 2.

Table 1- Values of the parameters used in calculation resistivity for a-Si

Material Silicon a-Si	Values of the parameters		
Resistivity Calculation	$Log_{e}A = 0.016$	$\alpha = 0.008$	$\beta = 0.029$

Table 2- Values of the parameters used in calculation resistivity for a-Si: H

Material Silicon a-Si : H	Values of the parameters		
Resistivity Calculation	$Log_{e}A = -0.056$	$\alpha = -0.026$	$\beta = -0.145$

A comparison of the present calculations with the experimental results [4] show that the deviation of theoretical value from the measurement is nowhere greater than 3% except in the neibhourhood of 1-2 kbar. From this, it appears that the assumptions on which our results are based may throw some light on the processes responsible for pressure induced variation in electrical resistivity of amorphous solids. It may be noted that Lazarus [4] in his concluding remarks has not clearly identified any of the pressure dependent physical processes, which may be operative in these amorphous semiconductors because of the limited temperature range available for the experimental investigations. Further, the information about the nature and content of the impurity in the samples used for measurements is also not available.

3.2 Germanium

In the present work the calculations made for this semiconductor have been compared with the experimental results of Paul and Brooks [9]. However, they have not carried out any resistivity measurements on this material. Here it may also be pointed out that the experiments on resistivity measurements were carried out by Paul and Brooks. Due to this, the parameters obtained from the numerical analysis of the band-gap (Eg) results by Goni et al [10] have been used to study the pressure induced resistivity of Ge as measured by Paul and Brooks [9].

The present results on pressure coefficient of band gap energy $(4.5 \times 10^{-6} \text{eV/bar})$ are comparable with the same quantity obtained experimentally $(5 \times 10^{-6} \text{eV/bar})$. However the experimental results obtained by Paul and brooks [9] were not in agreement with the results of Goni et al [10] $(12.1 \times 10^{-6} \text{eV/bar})$. The present work also includes the analysis of data published by Goni et al [10]. The theoretical values of the resistivity have been plotted in Figure 3 along with the experimental results. Both the theoretical results are in reasonable agreement with the measured values as it is clear from the Figure 3. The parameters used in the calculation are mentioned in Table 3 and according to formula equation (2).



Fig. 3- Variation of resistivity with pressure for a sample of n-type germanium at $296^0 \rm K$

Table 3- Values of the parameters used in calculation resistivity for germanium

Material Germanium (Ge)	Values of the parameters		
Resistivity Calculation	$\log_{e} A = 3.76$	α= 0.15	β= -1.37

3.3 Selenium

Selenium is other group material with a direct band gap in n-type conduction. It is used in selenium rectifiers. The effects of pressure on the optical edge of selenium have been studied by Balchan and Drickamer [11]. It was found that selenium approaches to metallic state near about 130 Kbar. Balchan and Drickamer have also carried out the resistance versus pressure measurements for selenium. It was found that selenium shows a sharp drop of about 2 to 3 orders of magnitude at 130 to 135 Kbar. Since the resistance and optical edge studies have been made by the same group, one can, therefore, test the applicability of Equation (2) for selenium.

Numerical studies for the electrical resistance against pressure have been made with the Equations (2) and the results have been compared with the measurements of Balchan and Drickamer in Figure 4 respectively. The numerical values of the parameters used in the calculations are listed in Table 4. The obtained values of the parameters have been utilized to estimate the expected pressure for metallization of selenium. This estimated pressure comes out to be 110 K bar which is in close agreement with the predicted value of 130 K bar.





Fig. 4- Relative resistance versus pressure for selenium

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