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Transport phenomena of $SmSe_{1-x}As_x$

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Abstract. Results are presented on the measurements of unit cell parameter and electrical resistivity under pressure on $SmSe_{1-x}As_x$ for $x = 0.1$, 0·2, 0·3 and 0·4. The electrical resistivity values are found to be decreasing with increase of pressure and also with increase of arsenic concentration. The semiconductor to metallic transition is induced by chemical alloying of SmSe with SmAs similar to that observed under pressure. The electrical resistivity values are also calculated which are in good agreement with the experimental values. In this calculation, the carrier mobility is of negative sign and so the sample $SmSe_{1-x}As_x$ is found to be *n*-type semiconductor.

Keywords. $SmSe_{1-x}As_x$; lattice parameter; electrical resistivity; semiconductor to metal transition; high pressure.

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1. Introduction

Monochalcogenides of divalent Sm, Eu and Yb crystallize in the NaCl structure and are found to be semiconductors [1]. Because of the smaller atomic volume in the trivalent state, pressure in general induce a transition from the divalent semiconducting state to trivalent metallic state [2], which can also be induced at room temperature and pressure by chemical alloying. To study the effect of alloying SmAs with SmSe [3], we have already reported [4] the electrical conductivity measurements and the results of X-ray diffraction studies on $SmSe_{1-x}As_x$ for $x = 0{\cdot}1$ and 0·4. The present study has been undertaken to closely examine the behaviour of electrical resistivity under pressure and lattice parameter variation between these two concentrations.

2. Experimental methods

X-ray powder diffraction studies on $SmSe_{1-x}As_x$ for $x = 0{\cdot}2$ and 0·3 have been carried out using Cukα radiation produced by a rotating anode X-ray generator. The sample had expected NaCl structure. Lattice parameters (table 1) obtained from six *d*-values by least square method are in good agreement with the reported values [5].

Electrical resistivity measurements has been carried out by using four-probe method [6] in Bridgemann anvil set-up, with anvils made of EN24 (AISI4340) alloy steel (Composition: C 0·04%, Mn 0·60%, Ni 1·55%, Cr 1·1%) hardened to RC60. The anvil face was 10 mm in diameter and had a tapering angle 10°. The pressure medium was steatite of 0·2 mm dia. The gaskets were pyrophyllite discs of 10 mm dia. A hydraulic press was used to apply the force.

From the electrical resistivity measurements, impurity activation energy [3, 7] ΔE

Table 1. Experimental and theoretical results of $SmSe_{1-x}As_x$.

	a in Å				
x	Present study	Reported	ΔE in eV	ρ experimental Ω-metre	ρ calculated Ω-metre
0·0	—	6·20	0·440	30[Ref. 7]	14·3
0·1	$6·18 \pm 0·02$	6·15	0·120	$1·2528 \times 10^{-2} \pm 0·00010$	$1·333 \times 10^{-2}$
0·2	$6·03 \pm 0·02$	6·05	0·074	$1·3265 \times 10^{-3} \pm 0·00009$	$7·351 \times 10^{-3}$
0·3	$5·99 \pm 0·01$	5·98	—	$2·2510 \times 10^{-4} \pm 0·00001$	—
0·4	$5·94 \pm 0·02$	5·94	—	$1·2005 \times 10^{-4} \pm 0·00001$	—

	Calculated parameters			
x	m^* in kg	n	ε	u in $m^2V^{-1}s^{-1}$
0·0	$4·794 \times 10^{-31}$	$1·804 \times 10^{21}$	4·023	$-2·417 \times 10^{-4}$
0·1	$2·108 \times 10^{-31}$	$2·671 \times 10^{23}$	5·108	$-1·753 \times 10^{-3}$
0·2	$1·370 \times 10^{-31}$	$3·428 \times 10^{23}$	5·244	$-2·477 \times 10^{-3}$

which is equal to αp_0 can be deduced. Here, α is the rate of closing of energy gap with pressure given by

$$\alpha = \frac{d\Delta Eg}{dp} = kT\left[\frac{d \ln \rho}{dp}\right] \tag{1}$$

and p_0 is the minimum pressure needed for the complete conversion of Sm^{2+} into Sm^{3+}, characterized in a sharp bending over and saturation effect conductivity in the $\ln\rho$-P plot [3].

3. Estimated electrical resistivity

The electrical resistivity has been theoretically calculated using the lattice constant and impurity activation energy. The Drude's model [8] defines the electrical conductivity σ which is the reciprocal of the electrical resistivity as

$$\sigma = 1/\rho = neu \tag{2}$$

where n is the carrier density, e the electron charge and u is the carrier mobility. The carrier density [9] n can be calculated by the formula

$$n = \frac{2(2\pi m^* kT)^{3/2}}{h^3} \exp\left[-\frac{\Delta E}{2kT}\right] \tag{3}$$

here m^* is the effective mass, ΔE impurity activation energy, k Boltzmann constant,

h the Plancks constant and T the temperature. The effective mass [10] can be given in terms of lattice parameter a and impurity activation energy ΔE as

$$\frac{m_0}{m^*} = 1 + \frac{2h^2}{m_0 a^2 \Delta E}. \tag{4}$$

Where m_0 is the electron rest mass. Then, the carrier mobility u can be determined [9] from the expression

$$u = \frac{3\varepsilon^2}{16\pi^2 m^* [\ln(1+x) - x/(1+x)]} \left[\frac{h}{e}\right]^3. \tag{5}$$

Here ε is the dielectric constant [9] which is given by

$$\varepsilon = \left[\frac{13{\cdot}53}{\Delta E}\frac{m^*}{m_0}\right]^{1/2} \tag{6}$$

and

$$x = \left[\frac{h}{e}\right]^2 \left[\frac{e}{m^*}\right] \left[\frac{3N}{8\pi}\right]^{1/3} \tag{7}$$

Where N is the impurity concentration given by

$$N = \frac{n^2}{2\left[\frac{2\pi m^* kT}{h^2}\right]^{3/4} \exp\left[-\frac{\Delta E}{2kT}\right]}. \tag{8}$$

Thus, the value of electrical resistivity at room temperature and pressure has been calculated by substituting n and u in eq. (3) for various values of x. The results are given in table 1. SmSe is characterized as [11] n type semiconductor. In this calculation the calculated mobility is of negative sign and therefore $SmSe_{1-x}As_x$ must be of n type semiconductors.

4. Conclusion

X-ray diffraction study on $SmSe_{1-x}As_x$ for $x = 0{\cdot}1$, $0{\cdot}2$, $0{\cdot}3$ and $0{\cdot}4$ shows that the sample is having expected NaCl type structure. The lattice parameters obtained for the samples are in good agreement with the reported values. The arsenic substitution in SmSe for Se causes the valence transition from Sm^{2+} to Sm^{3+}. The transition starts at $x = 0{\cdot}1$ and is nearly completed at about $x = 0{\cdot}4$. The behaviour of electrical resistivity of the samples as a function of pressure is shown in figure 1. The electrical resistivity decreases continuously with increase of pressure. From the resistivity measurements, impurity activation energy has been determined. The resistivity decreases continuously with increase of arsenic concentration similar to the behaviour observed under pressure. These lead to a conclusion that the semiconductor to metallic transition can be induced by chemical alloying SmSe with SmAs similar to that induced under pressure. The sample is in divalent semiconducting state at ambient pressure and temperature, and goes to trivalent metallic state under pressure at room temperature. As a function of arsenic concentration, $SmSe_{1-x}As_x$ is in semiconducting state at lower values of x and metallic state at about $x = 0{\cdot}4$. Then the electrical

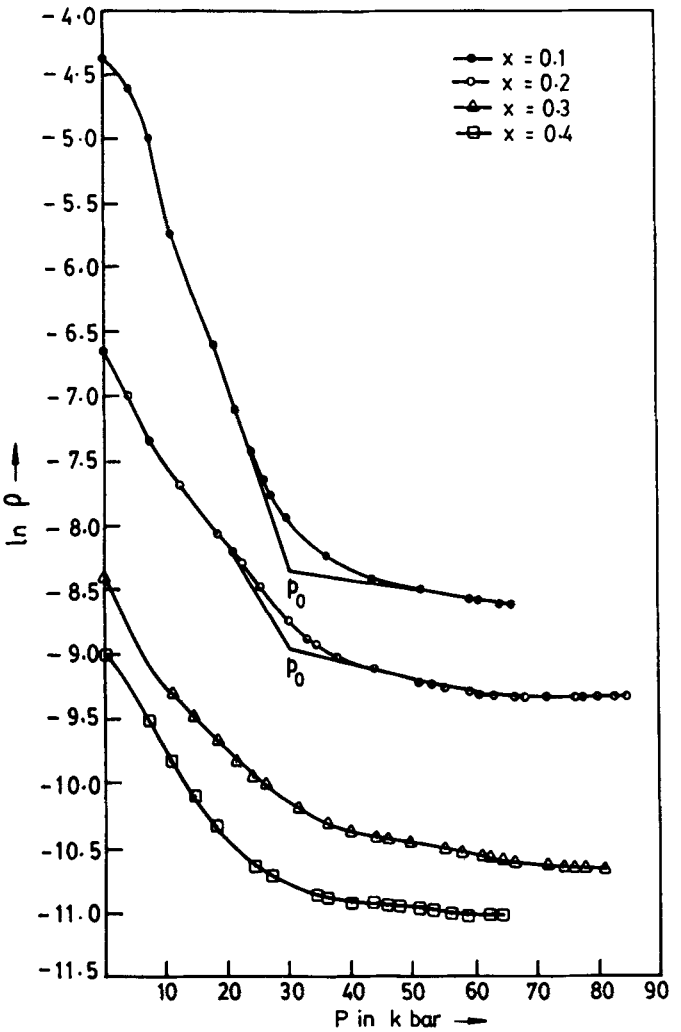

Figure 1. The behaviour of electrical resistivity of $SmSe_{1-x}As_x$ as a function of pressure.

resistivity values at ambient temperature and pressure are calculated using Drude's model for $x = 0{\cdot}0$, $0{\cdot}1$ and $0{\cdot}2$ which are in agreement with the experimental values. This method is applicable only to semiconductors and not to metals because of the dependence of the energy gap. Since the ρ values are approaching nearer to metallic state for $x = 0{\cdot}3$ and $0{\cdot}4$, this method is not applicable. The calculated effective mass, carrier density, carrier mobility and dielectric constant are given in table 1. It is notable that the calculated carrier mobility is of negative sign which leads to a conclusion that the sample is of n type semiconductor. The values of lattice constant, impurity activation energy and experimental as well as calculated electrical resistivity values are given in table 1. They are fairly in good agreement.

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