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Research paper

Effect of La-concentration (x) on some physical properties of $La_xSm_{1-x}S$ (x = 0, 0.1, 0.25 and 0.35) alloys

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Abstract

In the present work, we studied the effect of the incorporation of Lanthanum (La) atoms into Samarium monosulfide (SmS) small gap mag-netic semiconductor birary compound. So some physical properties of pure (SmS) and La-doped SmS compound $La_xSm_{1-x}S$ (x = 0.1, 0.25 and 0.35) ternary alloys) were obtained. We found that the longitudinal wave velocity of $La_xSm_{1-x}S$ ternary alloys decreases mono-tonically and non-linearly with increasing La-concentration (x) from 0 to 35%, while the transverse and average elastic wave velocities, Debye tem-perature and Vickers Hardness for $La_xSm_{1-x}S$ (x = 0, 0.1, 0.25 and 0.35) ternary alloys change non-monotonically and varied non-linearly with increasing La-concentration (x). For LaxSm1-xS (x = 0.1, 0.25 and 0.35) ternary alloys, the lattice parameters and the elastic constants used here are taken from the work of Schärer and Wachter (Solid State Communications, Vol. 96, No. 7, (1995), pp. 497–501), while for SmS divalent chalcogenide birary compound, the elastic constants used here are taken from the book edited by Sirdeshmukh et al. (D. B. Sirdeshmukh, L. Sirdeshmukh, K. G. Subhadra, Micro-and macro-properties of solids, Springer-Verlag Berlin Heidelberg, 2006, page 269). The Debye temperature was calculated using two different approches (Debye's approch and Blackman's approch) To the best of author knowledge, there is no any data in the literature on the Debye temperature and the minimum thermal con-ductivity for $La_xSm_{1-x}S$ (x = 0.1, 0.25 and 0.35) ternary alloys to make comparaison.

Keywords: *Elastic Constants; Elastic Wave Velocity; $La_xSm_{1-x}S$ (X = 0.1, 0.25 and 0.35) Ternary Alloys; Debye Temperature.*

1. Introduction

Chalcogenides are the compounds of the heavier chalcogens (sulfides, selenides, and tellurides) [1]. These compounds would afford a wide range of applications. Using the pseudopotentials, Density Functional Theory (DFT) method, Joshi [1] has studied the high-pressure phase transition of the lanthanum monochalcogenides LaX (X = S, Se, Te), while Okba and Mezouar [2] have investigated some physical parameters of calcium chalcogenides at high pressures using semi-empirical approach.

Until now, reported literature showed very little attention has been paid to study the physical properties of SmScompound and $Sm_xLa_{1-x}S$ (x = 0.9, 0.75, 0.65) ternary alloys is still to be discussed [3-6] in comparison with these reported for other materials [7-27].

Using the angular dispersion of the velocity of the surface acoustic phonons in the (100)-oriented plane and the measured bulk moduli, Schärerand Wachter [3] have calculated all elastic constants and Poisson's ratio of $Sm_xLa_{1-x}S$ (x = 0.9, 0.75, 0.65) ternary alloys, and they found also that the values of the elastic constant C_{12} are negative for all these alloys.

Jha and Sanyal [4] have investigated the phonon dispersion curves (PDC) and the phonon density of states (PDOS) for $Sm_xLa_{1-x}S$ (x = 0.9, 0.75, 0.65) alloys using a lattice dynamical model theory which includes the breathing motion of valence electrons of rare earth ions. Based on the breathing shell model (BSM), and they conclude that there are phonon anomalies in these ternary alloys.

Arya and Aynyas[5] have studied the second order elastic constants (SOEC), third order elastic constants (TOEC) and the high-pressure phase transition of $Sm_xLa_{1-x}S$ (x = 0.9, 0.75, 0.65) ternary alloys using the modified inter-ionic potential theory (MIPT). Arya and Aynyas[5] found the following phase transition pressures: 49.25 GPa for $Sm_{0.9}La_{0.1}S$ alloy, 55 GPa for $Sm_{0.75}La_{0.25}S$ alloy, and 63 GPa for $Sm_{0.65}La_{0.35}S$ alloy, respectively. However, to our knowledge, no thorough investigations in to the Debye temperature of La_xSm_{1-x}Salloys have been carried out up to date. For this reason, some physical properties of La_xSm_{1-x}Salloys are carefully examined in this study. So in the present work, we studied the effect of the incorporation of Lanthanum (La) atoms in SmScompound.SmS is a semiconductor with a very small gap of 0.1 eV between the 4f and 5d band shows intermediate valence at normal pressure [5]. So some physical properties of $La_xSm_{1-x}S$ (x = 0, 0.1, 0.25 and 0.35) ternary alloys were obtained and discused. For $La_xSm_{1-x}S$ (x = 0.1, 0.25 and 0.35) alloys, the experimental lattice parameters and the elastic constants used here are taken from the work of Schärerand Wachter [3], while for SmS compound, the elastic constants are taken from the work of Sirdeshmukh et al [28].

2. Theory and discussion of the results

The requirement of mechanical stability in a cubic crystal leads to the following restrictions on the elastic constants, $(C_{11} - C_{12}) > 0$, $C_{11} > 0$, $C_{44} > 0$, $(C_{11} + 2C_{12}) > 0$ [29-32]. The elastic constants C_{ij} in table 2 of Schärerand Wachter [3] obey these stability conditions. Cauchy's pressure ($Cp = C_{12} - C_{44}$) is an index for determining the ductile/brittle nature of compounds, where positive values of Cp correspond to ductile materials, while negative values of Cpindicales the brittleness, i.e the material will be non-metallic or with directional bonding [33, 34]. The elastic constants in table 2 of Schärerand Wachter [3] meaning that Cp is negative for $Sm_xLa_{1-x}S$ (x = 0.9, 0.75, 0.65) ternary alloys reflecting that all these materials are expected to be brittle in their behaviours.

Using the lattice parameters and the elastic constants of Schärerand Wachter [3] for $La_xSm_{1-x}S$ (x = 0.1, 0.25 and 0.35) ternary alloys, and the elastic constants are taken from the work of Sirdeshmukh et al [28] for Samarium monosulfideSmSbirarysemiconducting compound, the values of the longitudinal (v_l), transverse (v_t) andaverage (v_m) elastic wave velocities and Debye temperature (θ_D) for $La_xSm_{1-x}S$ (x = 0, 0.1, 0.25 and 0.35) ternary alloys are presented in Table 1. For more details on the calculation of v_l, v_t, v_m and θ_D for the aggregate polycrystalline solids from Debye's approch, plrase see the refrences [35-38]. In cubic systems, θ_D can be expressed in terms of the elastic constants C_{ij} and the mass density ρ using Blackman'sapproch, which is given by the following expression [39-40]:

$$\theta_D^3 = \frac{3.15}{8\pi} h^3 k^{-3} \left(n\rho^{-3/2} V_a^{-1}\right)\left(C_{11} - C_{12}\right)^{1/2}\left(C_{11} + C_{12} + 2C_{44}\right)^{1/2}\left(C_{44}\right)^{1/2} \quad (1)$$

Where h is the Planck's constant, k is the Boltzmann constant, n is the number of atoms in unit cell of volume V_a, and ρ is the density.

Table 1: Masse Density ρ, Longitudinal, Transverse and Average Elastic Wave Velocities and Debye Temperature of $La_xSm_{1-x}S$ (X = 0.1, 0.25 and 0.35) Ternary Alloys in Comparison with Other Available Data [28], *Using Debye's Approch, **Using Blackman's Approch

Material	M (g/mol)	ρ (kg/m^3) [3]	v_l (km/s)	v_t (km/s)	v_m (km/s)	θ_D(K)
SmS	182.43	5706	4.040	2.454	2.711	271*, 300**, 268 [28]
$La_{0.1}Sm_{0.9}S$	181.28	5761	3.791	2.571	2.804	281*, 306**
$La_{0.25}Sm_{0.75}S$	179.56	5911	3.300	2.528	2.705	275*, 289**
$La_{0.35}Sm_{0.65}S$	178.42	5908	3.175	2.508	2.668	272*, 281**

The values of the longitudinal (v_l), transverse (v_t) andaverage (v_m) elastic wave velocities and Debye temperature (θ_D) for $La_xSm_{1-x}S$ (x = 0, 0.1, 0.25 and 0.35) ternary alloys are also traced in Figure 1.

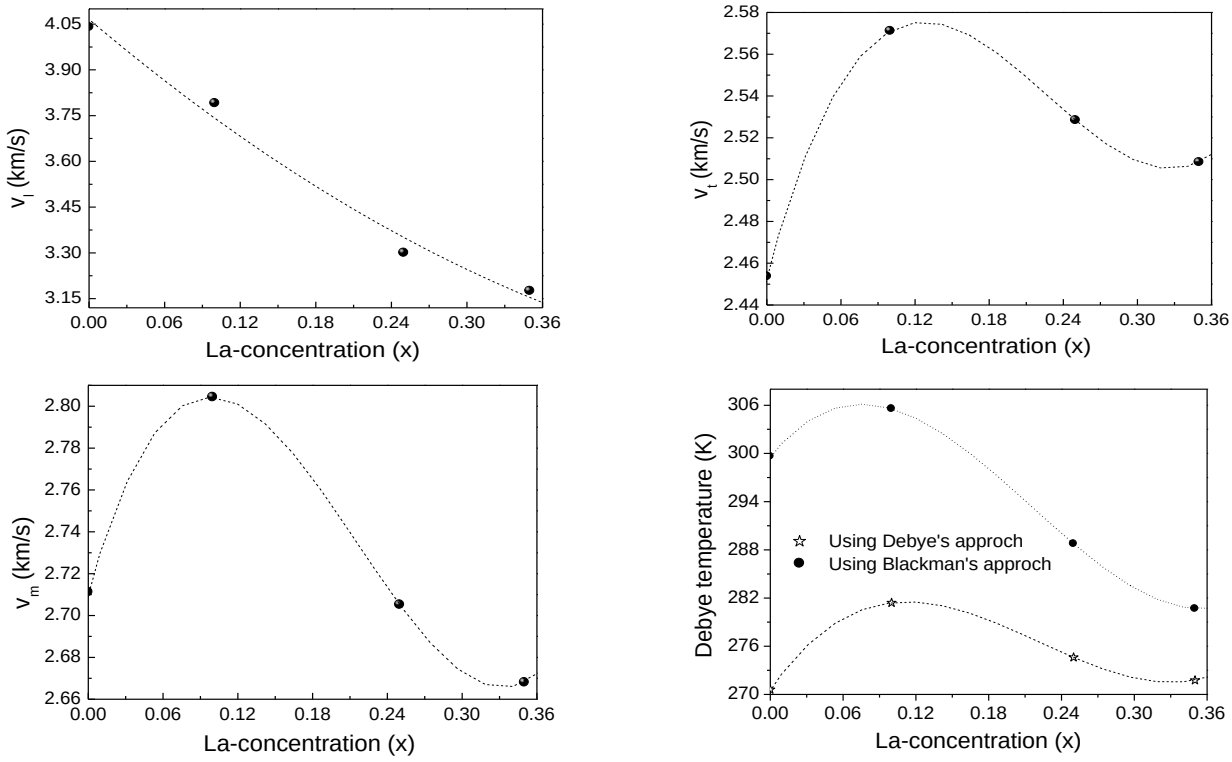

Fig. 1: Influence of La-Concentration on the Elastic Wave Velocities and Debye Temperature of $La_xSm_{1-x}S$ (x = 0.1, 0.25 and 0.35) Alloys.

From the results reported in Table 1, it is seen that the values of the Debye temperature obtained from Blackman'sapproch is higher than these calculated from Debye's approch. In addition, for SmSbirary compound, the deviation on the θ_D between our result (271 K) and that (268 K) of Sirdeshmukh et al [28] using the same approch is only 1.12%, and a good agreement is obtained. A material would have high value of high-temperature superconductivity Tc, provided its θ_D is large [41]. From the curves of Figure 1, it is seen that the longitudinal wave velocity of $La_xSm_{1-x}S$ (x = 0, 0.1, 0.25 and 0.35) decreases monotonically and non-linearly with increasing La-concentration (x), while the transverse and average elastic wave velocities and Debye temperature change non-monotonically and vary non-linearly with increasing La-concentration (x). Because the vibrational excitation arises solely from acoustic modes at low temperature, so, the Debye temperature calculated from elastic constants is the same as that determined from specific heat measurements [42].

If one dimension of the solid changed, other its dimensions need to be changed to keep the volume constant. The Poisson's ratiovis expressed as a function of Young'smodulus E andshear modulusG as follows: υ = (E/2G) - 1 [43]. We found the values of the Poisson's

ratiov: 0.21 for SmS, 0.07 for $La_{0.1}Sm_{0.9}S$, - 0.21 for $La_{0.25}Sm_{0.75}S$ and - 0.33 for $La_{0.35}Sm_{0.65}S$, respectively. The negative sign of the Poisson's ratiov was also obtained in the work of Schärerand Wachter [3] in $\langle 100 \rangle$-direction.

The hardness has a significant effect on the applications of the functional materials [44]. If the elastic moduli of the aggregate polycrystalline solids are known, it is possible to use them to calculate their hardness and several other paramters [45-50]. The Vickers hardness H_V and the shear modulus G are related by the empirical formula given as: $H_V = 0.1475 \times G$ [51, 52]. It is well known that the microhardness of a material change considerably as a function of dislocation density [53]. The values estimated at room temperature of the shear modulus G and the Vickers hardness H_V for $La_xSm_{1-x}S$ (x = 0, 0.1, 0.25 and 0.35) alloys depending on the doping concentration of La are also traced in Figure 2. From the curves of Figure 2, it is seen that the Vickers hardness H_V of $La_xSm_{1-x}S$ (x = 0, 0.1, 0.25 and 0.35) ternary alloys change also non-monotonically and vary non-linearly with increasing La-concentration (x). Our data's optimal fits for $La_xSm_{1-x}S$ (x = 0, 0.1, 0.25 and 0.35) alloys conform to the polynomial equations:$G= 34.4 + 63\ x -297.3\ x^2 + 400.7\ x^3$ (with G in GPa) and $H_V = 7.6 + 28.7\ x - 134.5x^2 + 196.4\ x^3$ (with H_V in GPa), respectively. The values of G and $H_V$forSmS binary compound seem also to be the smallest ones as compared to those for $La_xSm_{1-x}S$ (x = 0.1, 0.25 and 0.35) alloys.

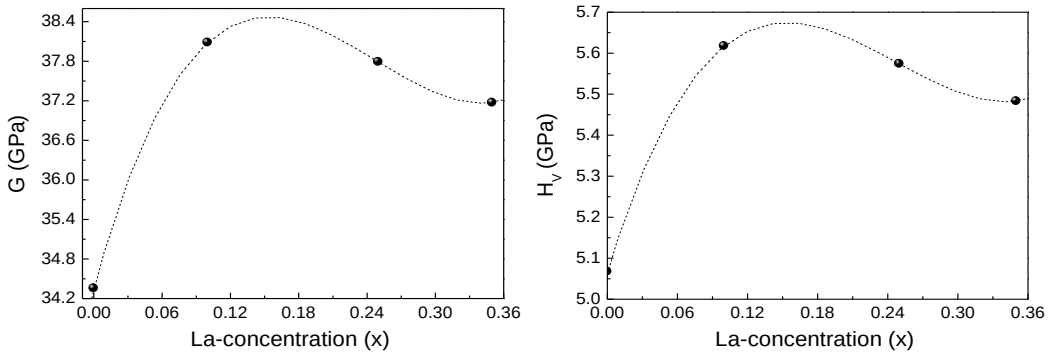

Fig. 2: Influence of La-Concentration (x) on the Isotropic Shear Modulus G and Vickers Hardness H_V of $La_xSm_{1-x}S$ (x = 0.1, 0.25 and 0.35) Alloys.

The combination of the bulk modulus B and the elastic constant C_{44} can be used to evaluate a compound's machinability through the machinability index $\mu_M = B/C_{44}$ [54]. μ_M offers a value that indicates the level of ease or diffiulty in machining a specific compound, involving processes such as cutting or shaping it into different forms [54]. The values estimated at room temperature of μ_M for $La_xSm_{1-x}S$(x = 0, 0.1, 0.25 and 0.35) depending on x of La-concentration (x) are also traced in Figure 3. It is seen that the machinability index μ_M of $La_xSm_{1-x}S$(x = 0, 0.1, 0.25 and 0.35) alloys decreases monotonically and non-linearly with increasing x.

Fracture toughness K_{IC} plays a pivotal role in the design and selection of materials [55-58]. For many covalent and ionic materials, the fracture toughness K_{IC} has been calculated using the following empirical expression $K_{IC} = V_0^{1/6}(B/G)^{1/2}G$ [55-58], where V_0 is the atomic volume (given in m^3), B is the bulk modulus and G is the shear modulus (both B and G are given in MPa). The values of the fracture toughness K_{IC} for $La_xSm_{1-x}S$ (x = 0, 0.1, 0.25 and 0.35) ternary alloys are ploted in Figure 3.

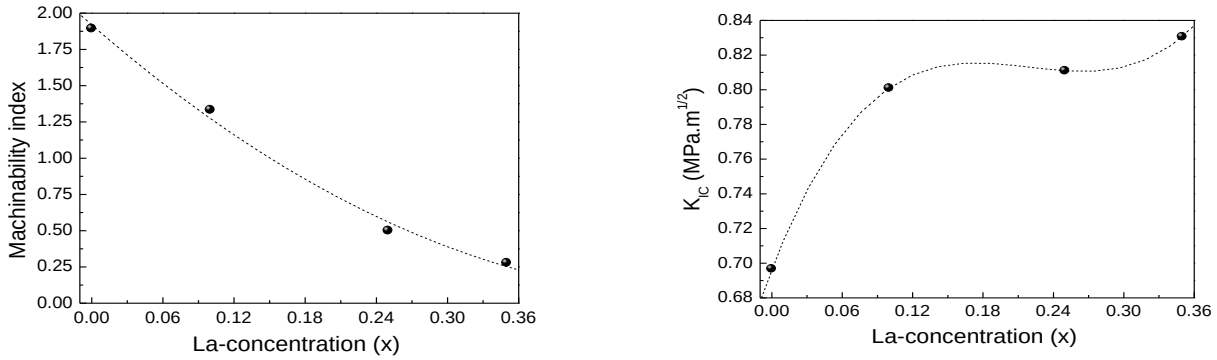

Fig. 3: Influence of La-Concentration (x) on the Machinability Index and The Fracture Toughness K_{IC} of $La_xSm_{1-x}S$(x = 0.1, 0.25 0.35) Alloys.

Our data's optimal fit of the fracture toughness K_{IC} for $La_xSm_{1-x}S$(x = 0, 0.1, 0.25 and 0.35) alloys as a function of La-concentration (x) conforms to the third order polynomial equation: $K_{IC} = 0.70 + 1.45\ x - 8.33\ x^2 + 12.64\ x^3$ (with K_{IC} in MPa.$m^{1/2}$).

In this section of the present work, we try to estimate the minimum thermal conductivity (κ_{min}) of $La_xSm_{1-x}S$ (x = 0, 0.1, 0.25 and 0.35) alloys. κ_{min} of some ceramic materials were calculated by Clarke [59]. Based on this model which suggested that the theoretical minimum conductivity could be calculated after replacing different atoms by an equivalent atom with a mean atomic mass of M/n [60], [61]:

$$\kappa_{\mathbf{min}} \rightarrow k_B \nu_m \left(M / ngN\right)^{-2/3} \tag{2}$$

where k_B is the Boltzmann's constant, υ_m is the average sound velocity, N is the Avogadro's number, g is the density, M is the molecular weight, and n is the number of atoms in the molecule.

Our numerical estimation of the κ_{min} for $La_xSm_{1-x}S$ (x = 0, 0.1, 0.25 and 0.35) alloys are: 0.42 W/K.m for SmS, 0.44 W/K.m for $La_{0.1}Sm_{0.9}S$, 0.44 W/K.m for $La_{0.25}Sm_{0.75}S$ and 0.45 W/K.m for $La_{0.35}Sm_{0.65}S$, respectively. It has been proven that material having higher Debye temperature, possissing greater wave speed velocity and greater thermal conductivity, and vice versa [62-64].

3. Conclusion

In conclusion, we made a study on the effect of the incorporation of Lanthanum-atoms into SmS semiconductor. In consequence some physical and mechanical properties of SmS binary semiconductor and $La_xSm_{1-x}S$ (x = 0.1, 0.25 and 0.35) ternary alloys were estimated at room temperature and analyzed. We found that the longitudinal wave velocity of $La_xSm_{1-x}S$material decreases monotonically and non-linearly with increasing La-concentration (x), while the transverse and average elastic wave velocities and Debye temperature for $La_xSm_{1-x}S$ alloys change non-monotonically and vary non-linearly with increasing La-concentration (x). The aggregate Poisson's ratiowas found positive for both for SmS and $La_{0.1}Sm_{0.9}S$ alloy and negative for both $La_{0.25}Sm_{0.75}S$ and $La_{0.35}Sm_{0.65}S$ ternary alloys.
To the best of author knowledge, there is no any data in the literature on the Debye temperature, Vickers hardness, fracture toughness, and the minimum thermal conductivity for $La_xSm_{1-x}S$ (x = 0.1, 0.25 and 0.35) to evaluate our obtained results and make comparaison.

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