Global Journal of Science Frontier Research
Physics & Space Science
Volume 12 Issue 1 Version 1.0 January 2012
Type : Double Blind Peer Reviewed International Research Journal
Publisher: Global Journals Inc. (USA)
Online ISSN: 2249-4626 & Print ISSN: 0975-5896

Study of High Pressure Structural, Mechanical and Thermal Properties of $SrS_{1-x}Se_x$, $SrS_{1-x}Te_x$ and $SrSe_{1-x}Te_x$ Ternary Alloys

By Purvee Bhardwaj
Barkatullah University, Bhopal, India

Abstract - We have developed a new model to study the structural, mechanical and thermal properties of $SrS_{1-x}Se_x$, $SrS_{1-x}Te_x$ and $SrSe_{1-x}Te_x$ ternary alloys. This model includes the Coulomb interaction, TBI interaction, vander Waal interaction overlap repulsive interactions extended up to the second neighbour ions and covalent interaction. The variation of Gibb's free energy, phase transition pressure and the bulk modulus from the concentration using Vegard's law were observed for the three alloys. Our calculated results have revealed reasonably good agreement with the available experimental data on the phase transition pressures and volume collapse. In addition we have calculated other mechanical and thermal properties.

Keywords : Strontium chalcogenides, Volume collapse, Elastic constants, Phase transition.

GJSFR-A Classification : FOR Code: 020304 ,020406

Study of High Pressure Structural, Mechanical and Thermal Properties of $SrS_{1-x}Se_x$, $SrS_{1-x}Te_x$ and $SrSe_{1-x}Te_x$ Ternary Alloys

Purvee Bhardwaj

Abstract - We have developed a new model to study the structural, mechanical and thermal properties of $SrS_{1-x}Se_x$, $SrS_{1-x}Te_x$ and $SrSe_{1-x}Te_x$ ternary alloys. This model includes the Coulomb interaction, TBI interaction, vander Waal interaction overlap repulsive interactions extended up to the second neighbour ions and covalent interaction. The variation of Gibb's free energy, phase transition pressure and the bulk modulus from the concentration using Vegard's law were observed for the three alloys. Our calculated results have revealed reasonably good agreement with the available experimental data on the phase transition pressures and volume collapse. In addition we have calculated other mechanical and thermal properties.

PACS No : 62.20.de, 62.20.dq, 62.50.-p, 64.00.00

Keywords : Strontium chalcogenides, Volume collapse, Elastic constants, Phase transition.

I. INTRODUCTION

The strontium chalcogenides SrX (X = S , Se and Te), together with other alkaline earth chalcogenides form a very important closed shell ionic system with the NaCl crystal structure at normal conditions. They are technologically important materials, with applications in the area of luminescent devices, radiation dosimetry, fast high-resolution optically stimulated luminescence imaging, and infrared sensitive devices [1–3]. Under higher pressure prior to metallization, they undergo a first order structural phase transition to the CsCl structure. Semiconductor alloys, which are solid solutions of two or more semiconducting elements, have important technological applications, especially in the manufacture of electronic and electro-optical devices [4-6]. One of the easiest ways to change artificially the electronic and optical properties of semiconductors is by forming their alloys. It is possible to combine two different compounds with different optical band gaps and different rigidities in order to obtain a new material with intermediate properties.

There are a number of theoretical works on these compounds concerning electronic band structure, structural phase stability, elastic properties, metallization process and optical properties [7–11]. For the band gap results, there are some discrepancies between different calculations. Recently, Dadsetani et. al. [1] have calculated the optical properties of SrS, SrSe and SrTe compounds using the full potential linearized augmented plane wave method (FP-LAPW). To the best of our knowledge no experimental or theoretical investigations of their ternary alloys have been appeared in the literature, therefore, the purpose of this paper is to study the structural, elastic, and thermodynamic properties as well as to investigate the disorder effects in these strontium alloys using the charge transfer mechanism.

Zimmer et. al. [4] investigated pressure volume relationships and structural transition in CaTe and SrTe at high pressure using X-ray diffraction. Their results show that SrTe transforms from B1 to B2 structure at 12 GPa. Luo. et. al. [5] studied the high pressure phase transformation and the equation of state of SrSe by X-ray diffraction using a synchrotron source. They reported a B1-B2 structural transition at 14.2 GPa with a volume reduction of 10.7%. Khenata et. al. [6] calculated the electronic band structures and the total energies of SrS, SrSe and SrTe in the B1 and B2 structures. They determined the transition and metallization pressure in these compounds.

Metallization is often described in terms of the single particle band and the unoccupied conduction band. The band gaps in these close shell insulating materials are expected to decrease with pressure until finally the empty d-type conduction band drops in energy below the top of the filled p-type valence bands. Saum et. al. [9] measured the fundamental optical absorption of SrS, Sr Se and SrTe in the energy range from 2.5 to 5.8 eV. Cheng Yan et al [10] investigated the transition phase and elastic properties of SrS from NaCl structure (B1) to CsCl structure using the ab-initio plane wave pseudopotential density functional theory and by the quasi-harmonic Debye model. Yang Xiao-Cui et al [11] investigated the structural stabilities and electronic properties of SrX (X=S, Se , T e) under high pressure using the first principles calculation based on density functional theory (DFT) with the plane wave basis.

Jha et al [12] reported the investigation of the pressure induced phase transition of BaSe, BaTe, SrSe, and SrTe, using a three-body potential approach. But, they ignored the van-der Waal and covalency effect. The ab initio full potential linearized augmented plane

---

Author : High Pressure Research Lab, Department of Physics, Barkatullah University, Bhopal-462026, India.
E-mail : purveebhardwaj@gmail.com Ph: +91-755-2487552, Fax +91-755-2677723

wave (FP-LAPW) method within density functional theory (DFT) was applied to study the effect of composition on the structural, electronic, optical and thermodynamic properties of $SrS_{1-x}Se_x$, $Sr\ S_{1-x}Te_x$ and $SrSe_{1-x}Te_x$ ternary alloys by S Labidi et al [13].

It is seen from the current literature that three body potential model (TBP) used and developed by Singh and coworkers [14-16] has been found to be remarkably successful in giving the unified description of the lattice dynamic, static elastic, optic, dielectric and photo elastic properties of ionic and semi conducting crystals. In this TBP model, the three body interactions owe their origin to the quantum mechanical foundation and also to the phenomenological approach in terms of the transfer (or exchange) of charge between the overlapping electron shells of the adjacent ions in solids. This TBP approach has been extended to include the Hafemeister-Flygare (HF) type [17] overlap repulsion operative upto the second neighbour ions for describing the lattice static and mechanical properties of binary ionic solids and alloys. Also, Tosi and coworkers [18] have demonstrated the significance of van der Waals (vdW) attraction due to the dipole-dipole (d-d) and dipole-quadruple (d-q) interactions to describe the cohesion in ionic solids. The van der Waal interactions are generally ignored in the first principle calculations. Besides, it is noted that Motida [19] has incorporated the effect of covalency to reveal the cohesive and lattice properties of partially ionic crystals.

II. Essentials of Theory and Computational Method

The natural consequence of application of pressure on the crystals is the compression, which in turn leads to an increased charge transfer (or three-body interaction effects) [14] due to the existence of the deformed (or exchanged) charge between the overlapping electron shells of the adjacent ions.

These effects have been incorporated in the Gibbs free energy ($G = \Phi + PV - TS$) as a function of pressure and three body interactions (TBI), which are the most dominant among the many body interactions. Here, Φ is the internal energy of the system equivalent to the lattice energy at temperature near zero and S is the entropy. At temperature T=0K and pressure (P) the Gibbs free energies for rock salt (B1, real) and CsCl (B2, hypothetical) structures are given by:

$$G_{B1}(r) = \phi_{B1}(r) + P_{B1}(Vr) \tag{1}$$

$$G_{B2}(r') = \phi_{B2}(r') + P_{B2}(Vr') \tag{2}$$

With V_{B1} ($=2.00r^3$) and V_{B2} ($=1.54r'^3$) as unit cell volumes for B_1 and B_2 phases respectively. The first terms in (1) and (2) are lattice energies for B_1 and B_2 structures and they are expressed as:

$$\begin{aligned}\phi_{B_1}(r) = {} & \frac{-\alpha_m z^2 e^2}{r} - \frac{(12\alpha_m z e^2 f_m(r))}{r} - \left[\frac{C}{r^6} + \frac{D}{r^8}\right] + 6b\beta_{ij}\exp\left[(r_i + r_j - r)/\rho\right] \\ & + 6b\beta_{ii}\exp\left[(2r_i - 1.414r)/\rho\right] + 6b\beta_{jj}\exp\left[(2r_j - 1.414r)/\rho\right]\end{aligned} \tag{3}$$

$$\begin{aligned}\phi_{B_2}(r') = {} & \frac{-\alpha'_m z^2 e^2}{r'} - \frac{(16\alpha'_m z e^2 f_m(r'))}{r'} - \left[\frac{C'}{r'^6} + \frac{D'}{r'^8}\right] + 8b\beta_{ij}\exp\left[(r_i + r_j - r')/\rho\right] \\ & + 3b\beta_{ii}\exp\left[(2r_i - 1.154r')/\rho\right] + 3b\beta_{jj}\exp\left[(2r_j - 1.154r')/\rho\right]\end{aligned} \tag{4}$$

With α_m and α'_m as the Madelung constants for NaCl and CsCl structure respectively. C (C') and D (D') are the overall vander Waal coefficients of B1 (B2) phases, β_{ij} (i,j=1,2) are the Pauling coefficients defined as $\beta_{ij} = 1 + (Z_i/n_i) + (Z_j/n_j)$ with Z_i (Z_j) and n_i (n_j) are the valence and the number of electrons of the i(j)th ion. Ze is the ionic charge and b (ρ) are the hardness (range) parameters, r (r') are the nearest neighbour separations for NaCl (CsCl) structure $f_m(r)$ is the modified three body force parameter which includes the covalency effect with three body interaction r_i (r_j) are the ionic radii of ions i (j).

These lattice energies consist of long range Coulomb energy (first term), three body interactions corresponding to the nearest neighbour separation r (r') (second term), vdW (vander Waal) interaction (third term), energy due to the overlap repulsion represented by Hafemeister and Flygare (HF) type potential and extended up to the second neighbour ions (fourth, fifth and sixth terms).

Covalency effects have been included in the second terms parameters of cohesive energies given by equation (3) and (4) in three-body interaction on the lines of Motida [19]. Now modified three body parameter $f_m(r)$ becomes

$$f_m(r) = f_{TBI}(r) + f_{\mathrm{cov}}(r) \tag{5}$$

$$f_{\mathrm{cov}}(r) = \frac{4V^{2}{}_{sp\sigma}e^{2}}{rE_{g}{}^{3}}$$

$$\frac{V_{sp\sigma}^{2}}{E_{g}^{2}} = \frac{1-e_{s}^{*}}{1\ 2}$$

$$E_{g} = E - I\,\frac{(2\alpha-1)e^{2}}{r} \qquad (6)$$

With $V_{sp\sigma}$ is the transfer matrix between the outer most P orbital of anion and lowest excited state of cation E_g is the transfer energy of electron from anion to cation. Denoting the static and optical dielectric constant ε_0 and ε respectively and the transverse optical phonon frequency at zone centre by ω_t, e_s represented as

$$(e_{s}^{*})^{2} = \frac{9\mu\,\omega_{t}^{2}(\varepsilon_{0}-\varepsilon_{\infty})}{4\pi N(\varepsilon_{\infty}+2)^{2}}$$

$$and \qquad (7)$$

$$\frac{(e_{s}^{*})^{2}}{(e)^{2}} = \frac{9v\mu\,\omega_{0}^{2}(\varepsilon_{0}-\varepsilon_{\infty})}{4\pi e^{2}(\varepsilon_{\infty}+2)^{2}}$$

Where ν denotes the unit cell volume: $2r^3$, r equilibrium value of the separation of the nearest neighbouring ions, ε_0 the static dielectric constants, μ reduced mass of the ions, and ω_0 the infrared dispersion frequency, these values have been taken from [19].

The values of derivatives of $f_m(r)$ obtained as

$$f_{m}(r) = f_{0}e^{-r/\rho} + f_{\mathrm{cov}}(r)$$ and its first derivative is

$$f_{m}{}'(r) = f{}'(r) + f{}'_{\mathrm{cov}}(r)$$

Where, various symbols have their usual meanings describe in our earlier paper [20-22]. The mixed crystals, according to the virtual crystal approximation (VCA) [23], are regarded as any array of average ions whose masses, force constants, and effective charges are considered to scale linearly with concentration (x). The measured data on lattice constants in $SrS_{1-x}Se_x$, Sr $S_{1-x}Te_x$ and $SrSe_{1-x}Te_x$ have shown that they vary linearly with the composition (x), and hence they follow Vegards law:

$$a\,(A\,B_{1-x}\,C_{x}) = (1-x)\,a\,(AB) + xa\,(AC) \qquad (8)$$

The values of these model parameters are the same for end point members. The values of these parameters for their mixed crystal components have been determined from the application of Vegards law to the corresponding measured data for AB and AC. It is instructive to point that the mixed crystals, according to the virtual crystal approximation, are regarded as an array of average ions whose masses, force constants and effective charges are considered to scale linearly with concentration. It is convenient to find the three parameters for both binary compounds. Furthermore, we assume that these parameters vary linearly with x and hence follow Vegards law:

$$b\,(A\,B_{1-x}\,C_{x}) = (1-x)\,b\,(AB) + xb\,(AC) \qquad (9)$$

$$\rho\,(A\,B_{1-x}\,C_{x}) = (1-x)\,\rho\,(AB) + x\rho\,(AC) \qquad (10)$$

$$f(r)\,(AB_{1-x}\,C_{x}) = (1-x)\,f\,(r)\,(AB) + xf\,(r)\,(AC) \qquad (11)$$

a) Thermo Physical Properties

In order to access the relative merit of the present potential we have calculated the molecular force constant (f), infrared absorption frequency (υ_0), Debye temperature (θ_D), Grunneisen parameter (γ) and ratio of volume expansion coefficient (α_v) to specific heat (C_v) at constant volume which are directly derived from the cohesive energy [20-22], $\Phi(r)$.

The compressibility is well known to be given by

$$\beta = \frac{3Kr_{0}}{f} \qquad (12)$$

in terms of molecular force constants

$$f = \frac{1}{3}\left[\phi_{kk'}^{SR}(r) + \frac{2}{r}\phi_{kk'}^{SR}(r)\right]_{r=r_{0}} \qquad (13)$$

With $\Phi_{kk'}{}^{SR}(r)$ as the short range nearest neighbour ($k\neq k'$) part of Φ (r) given by the last three terms in eq. (3) and (4). This force constant f leads to the infrared absorption frequency with the knowledge of the reduced mass (μ) of the oxide crystals.

$$\nu_{0} = \frac{1}{2\pi}\left(\frac{f}{\mu}\right)^{1/2} \qquad (14)$$

This frequency gives us the Debye temperature

$$\theta_{D} = \frac{h\nu_{0}}{k} \qquad (15)$$

With h and k as the Planck and Boltzman constants, respectively. The values of the Grunneisen parameter (γ), have been calculated from the relation

$$\gamma = -\frac{r_{0}}{6}\left[\frac{\phi'''(r)}{\phi''(r)}\right]_{r=r_{0}} \qquad (16)$$

We have calculated the ratio of the volume expansion coefficient (α_v) to the volume to specific heat (C_v) from its well known expression

$$\frac{\alpha_v}{C_v} = -\left[\frac{\phi'''(r)}{2r\phi''(r)}\right]_{r=r_0} \tag{17}$$

The thermal expansion coefficient (α_v) can be calculated with the knowledge of specific heat (C_v).

III. Results and Discussion

The Three Body potential described in the preceding section for NaCl (B_1) CsCl (B_2) structures contain three model parameters [b ρ, f(r)], namely range, hardness and three body interaction parameter. To calculate these parameters we employed the first and second order space derivatives of lattice energy and equilibrium condition. We have followed the technique of minimization of U_{B1} (r) and U_{B2} (r') at different pressures in order to obtain inter ionic separation r and r, for B_1 and B_2 phases respectively. We have evaluated the corresponding $G_{B1}(r)$ and $G_{B2}(r')$ and their respective differences $\Delta G = (G_{B1}(r) - G_{B2}(r'))$. The pressure at which ΔG approaches zero is the phase transition pressure (P_t).

Firstly, the structural properties of the binary compounds SrS, SrSe and SrTe in the rocksalt structure were analyzed. We model the alloys at some selected compositions with ordered structures described in terms of periodically repeated super cells with eight atoms per unit cell, for the compositions $x = 0.25, 0.5, 0.75$. The values of phase transition pressures of SrX mixed crytals for model-I and model-II at diffrent concentrations are given in Table-1. The values of phase tarnsition of model-I and model-II are compared with experimental and others data for end point members and psedoexperimental data for diffrent concentrations. The variations of Gibb's free energy change ΔG (KJ/mole) with concentration (x) are plotted in Fig 1. The Gibb's free energy change ΔG of SrX are dependent lineraly with concentration (x). The phase transition pressures of $SrS_{1-x}Se_x$, $SrSe_{1-x}Te_x$ and $SrS_{1-x}Te_x$ have been plotted with different concentration (x) in Fig. 2. We have compared our results with theoretical [3,5] and experimental results [6].

The first order phase transition involving a discontinuity in volume takes place at the transition pressure. Experimentally one usually studies the relative volume changes ($-\Delta V/V_0$) associated with the compressions. The discontinuity in volume ($-\Delta V/V_0$) at the transition pressure is obtained from the phase diagram. The negative sign shows compression in crystal. This is the characteristic of first order phase transition. The volume collapse of SrX mixed crystals are given in Table-1. The values of model-I and model-II of end point memers are compared with experiment and other theoretical data. Our values of model-I are better than other theoretical values. The volume collapse of SrX mixed crystals at diffrent concentrations are compared with psedoexperimental data.

Usually, in the treatment of alloy problems, it is assumed that the atoms are located at ideal lattice sites and the lattice constants of alloys should vary linearly with composition x according to Vegard's law [23], however, violations of Vegard's rule have been reported in semiconductor alloys both experimentally [3,5] and theoretically [6,12,13]. To test the mechanical stability of our model, we have computed the elastic properties of proposed materials.

To study the elastic behavior of strontium compounds we have studied second order elastic constants (SOECs) and their combinations. We have made further investigations from the variations of the bulk modulus $B [= (C_{11}+2C_{12})/3]$, the combination of SOEC elastic stiffness $C_L[=(C_{11}+C_{12}+2C_{44})/2]$ and the shear moduli $Cs [= (C_{11}-C_{12})/2]$. The values of these combinations for model-I and model-II are given in Table-2 at P=0 GPa. The values of the bulk modulus B are calculated for the compositions $x = 0.25, 0.5, 0.75$ by S Labidi et al [13] using the ab initio full potential linearized augmented plane wave (FP-LAPW) method within density functional theory (DFT). We have calculated the bulk modulus B at the same concentration for both the models and compared them with FP-LAPW results. Significant deviations of the bulk modulus from the linear concentration dependence have been plotted in Fig 3. Our results show that the bulk modulus decreases with an increase of the Se and Te concentration x which is same as S Labidi et al [13]. This suggests that as x increases from $x = 0$ to 1 the alloys become generally more compressible.

In order to investigate elasticity of SrX compounds in detail, we have used normalized elastic constants c_{ij} [24]. The value of c_{ij} is obtained by dividing a specific elastic constant by the bulk modulus

$$c_{ij} = c_{ij}/B = 3c_{ij}/(c_{11} + 2c_{12}).$$

Divided by the bulk modulus, the interatomic forces are normalized with an average restoring force of the system. At zero pressure, if a cubic crystal is elastically ideal, namely an isotropic Cauchy solid. The normalized elastic constants of $SrS_{1-x}Se_x$, $SrSe_{1-x}Te_x$ and $SrS_{1-x}Te_x$ have been summarized in Table-3.

Besides we have calculated thermo physical properties of SrX. The thermo physical properties provide us the interesting information about the substance. The Debye characteristic temperature θ_D reflects its structure stability, the strength of bonds between its separate elements, structure defects availability (dislocations in crystalline structure of mineral grains, pores, microcracks) and its density.

Compressibility is used in the earth science to quantify the ability of a soil or rock to reduce in volume with applied pressure.The calculated thermo physical properties have been listed in Table 4. Due to the lack of experimental data, we could not compare them with our results.

In view of the overall achievements, it may be concluded that there is reasonably good agreement of modified MTBP (Model-I) with the experimental values than computed from TBP (Model-II). The success achieved in the present investigation can be ascribed to the realistic approach of our model. The charge transfer effect seems to be of great importance at high pressure when the inter-ionic separation reduces considerably and the coordination number increases. For the study of the phase transitions in partially covalent chalcogenides, we have incorporated, probably for the first time, the effect of covalency in the TBP model along with the van der Waals interactions. The consistency of the results obtained from the TBI potential arose because the electron-shell deformation, when the nearest neighbour ions overlap, is enhanced under pressure. This supports our view of a partially ionic character and a charge transfer. It is thus obvious from the overall results that the present TBI mechanism is adequately suited for a description of the phase transition phenomena and mechanical properties, and we stress that the TBI gives a realistic representation of interionic interaction capable of explaining the elastic behaviour.

Finally, it may be concluded that the present modified interaction potential model (MIPM) has successfully predicted the phase transition pressures, associated volume collapses, elastic and thermophysical properties correctly for the present group of compounds. The inclusion of three body interactions with covalency effect has improved the prediction of phase transition pressures over that obtained from the two-body potential and TBI without covalency.

REFERENCES REFERENCES REFERENCIAS

1. M. Dadsetani and A. Pourghazi, Phys. Rev. B, 73 (2006), 195102-195109.
2. R. Khenata, H. Baltache M, Rerat M Driz. M, Sahnoun, B. Bouhafs, B. Abbar, Physica B, 371 (2006), 12-19.
3. H. G. Zimmer., H. Winze and K. Syassen, Phys. Rev.B, 32 (1985) 4066-4070; K. Syassen, Phys. Stat. Sol. (a)91 (1985) 11.
4. A. Chakrabarti, Phys. Rev.B, 62 (2000), 1806-1814.
5. Huan Luo, Raymond G. Green and Arthur L. Ruff, Phys. Rev. B, 49, (1994), 15341-15343.
6. Khenata R, Baltache H, Rerat M, Driz M. Sahnoun, M, Bouhafs, B, Abbar, B. Physica B 339 (2003) 208-215.
7. T.A. Grzybowski, L. Ruoff, Phys. Rev. B 27 (1983) 6502.
8. T.A. Grzybowski, L. Ruoff, Phys. Rev. Lett. 53 (1984) 489.
9. G.A. Saum, E.B. Hensley, Phys. Rev. 113 (1959) 1019.
10. Yan Cheng, Lai-Yu Lu, Ou-He Jia, Qing-Quan Gou, Commun. Theor. Phys. 49 (2008) 1611.j
11. Xiao-Cui Yang, Ai-Min Hao, Jie Yang, Yong-Hao Han, Gang Peng, Chun-Xiao Gao, Guang-Tian Zou, Chin. Phys. Lett. 25 (5) (2008) 807.
12. P.K. Jha, U.K. Sakalle, S.P. Sanyal, J. Phys. Chem. Solids 59 (1998) 1633.
13. S. Labidi, H. Meradji, M. Labidi, S. Ghemid, S. Drablia and F. El Haj Hassan, Physics Procedia 2 (2009) 1205–1212.
14. R.K. Singh, Phys. Reports 85 (1982) 259.
15. R.K. Singh Sadhna Singh, Phys. Rev. B 45 (1992) 1019.
16. R.K. Singh Sadhna Singh, Phase Transit. 15 (1989) 127.
17. Hafemiester D W and Flygare H F 1965 J. Chem. Phys. 43 795.
18. Tosi M P and Fumi F G 1962 J. Phys. Chem. Solids 23 359; Tosi M P 1964 Solid State Physics 16 1.
19. K. Motida, J. Phys. Soc. Jpn. 55 (1986) 1636.
20. Purvee Bhardwaj, Sadhna Singh and N. K. Gaur, Mat. Res. Bull. 44 (2009) 1366-1374.
21. Purvee Bhardwaj, Sadhna Singh and N. K. Gaur, J. Cetr. Euro. J. Phys. 6, 2 (2008) 223-229.
22. Purvee Bhardwaj, Sadhna Singh and N. K. Gaur, J. of Molecular Structure: THEOCHEM 897 (2009) 95-99.
23. R J Elliot and R A Leath, IIE 386 (1996).
24. Sadhna Singh and Purvee Bhardwaj J of Opto. and Advanced Material 12 (2010) 2261 – 2271.

CAPTIONS OF FIGURES

1. Gibb's free energy ΔG (kj/mole) with concentration (x) of $SrS_{1-x}Se_x$, $SrSe_{1-x}Te_x$ and $SrS_{1-x}Te_x$ respectively.
2. Phase transition pressure with concentration (x) of SrX solid squares (■), solid circles (●) solid triangles (▲), and represent for $SrS_{1-x}Se_x$, $SrSe_{1-x}Te_x$ and $SrS_{1-x}Te_x$ respectively.
3. Bulk modulus of SrX with concentration (x) solid squares (■), solid circles (●) solid triangles (▲), and represent for $SrS_{1-x}Se_x$, $Sr\,Se_{1-x}Te_x$ and $SrS_{1-x}Te_x$ respectively.

Table-1 : Phase transition and volume collapse of SrX at different concentration

Alloys/ Concentration	Phase Transition Pressure (GPa)				Volume Collapse (%)			
	Present		Expt.	Others	Present		Expt.	Others
	Model-I	Model-II			Model-I	Model-II		
SrS$_{1-x}$Se$_x$ 0	18.2	18.6	18^a	18.17^b	10.46	10.12	11.4^a	10.8^b
0.25	17.08	17.28	17.13^a	17.6^b	10.32	9.95	11.22^a	10.59^b
0.5	15.96	15.96	16.26^a	17.03^b	10.19	9.78	11.05^a	10.38^b
0.75	14.84	14.64	15.39^a	16.46^b	10.05	9.61	10.87^a	10.17^b
1	13.7	13.3	14.5	15.87^b	9.92	9.45	10.7^a	9.96^b
SrSe$_{1-x}$Te$_x$ 0	13.7	13.3	14.5^a	15.87^b	9.92	9.45	10.7^a	9.96^b
0.25	13.23	12.78	13.88^a	15.22^b	10.05	9.60	10.8^a	9.70^b
0.5	12.76	12.26	13.26^a	14.57^b	10.18	9.76	10.9^a	9.44^b
0.75	12.29	11.74	12.64^a	13.92^b	10.31	9.92	11.0^a	9.18^b
1	11.8	11.2	12^a	13.24^b	10.44	10.08	11.1^a	8.92^b
SrS$_{1-x}$Te$_x$ 0	18.2	18.6	18^a	18.17^b	10.46	10.12	11.4^a	10.8^b
0.25	16.6	16.7	16.5^a	16.94^b	10.455	10.11	11.32^a	10.33^b
0.5	15.0	14.9	15.0^a	15.71^b	10.450	10.10	11.25^a	9.86^b
0.75	13.4	13.05	13.5^a	14.48^b	10.445	10.09	11.17^a	9.39^b
1	11.8	11.2	12^a	13.24^b	10.44	10.08	11.1^a	8.92^b

a-ref [3,5], b-ref [6].

Table-2 : Bulk modulus and shear modulus of SrX at different concentration

Alloys/ Concentration	Bulk modulus (GPa)				Shear modulus (GPa)			
	Present		Expt.	Others	Present		Expt.	Others
	Model-I	Model-II			Model-I	Model-II		
SrS$_{1-x}$Se$_x$ 0	51.9	51.53	58^a	46.3^b	58.65	58.7	-	61.9^b
0.25	50.84	50.48	54.75^a	45.6^b	56.8	56.89	-	56.63^b
0.5	49.78	49.43	51.5^a	44.8^b	54.95	55.08	-	51.36^b
0.75	48.72	48.38	48.25^a	43.5^b	53.1	53.27	-	46.09^b
1	47.66	47.31	45^a	41.1^b	51.25	51.46	53.3^a	40.8^b
SrSe$_{1-x}$Te$_x$ 0	47.66	47.31	45^a	41.1^b	51.25	51.46	53.3^a	40.8^b
0.25	44.69	44.4	43.75^a	38.1^b	49.5	49.71	-	42.31^b
0.5	41.72	41.49	42.5^a	34.0^b	47.85	47.96	-	43.82^b
0.75	38.75	38.58	41.25^a	32.0^b	46.15	46.21	-	45.32^b
1	35.76	35.64	40^a	31.8^b	44.44	44.46	-	46.85^b
SrS$_{1-x}$Te$_x$ 0	51.9	51.53	58^a	46.3^b	58.65	58.7	-	61.9^b
0.25	47.87	47.56	53.5^a	41.6^b	55.1	55.14	-	58.13^b
0.5	43.84	43.59	49^a	37.5^b	51.55	51.58	-	54.37^b
0.75	39.81	39.62	44.5^a	33.5^b	48.0	48.02	-	50.61^b
1	35.76	35.64	40^a	31.8^b	44.44	44.46	-	46.85^b

a-ref [3,5], b-ref [13]

Table-3 : Normalized Elastic constants

Normalized elastic constants	SrS		SrSe		SrTe	
	Model-I	Model-II	Model-I	Model-II	Model-I	Model-II
C'_{11}	2.50	2.51	2.43	2.45	2.65	2.66
C'_{12}	0.246	0.238	0.283	0.274	0.171	0.168
C'_{44}	0.960	0.933	0.709	0.705	1.12	1.12

Table 4 : Thermo physical properties of SrX.

Crystal	***f*** **(10^4dyn/cm)**	**υ_0 (10^{12} Hz)**	**θ_D (K)**	**γ**	**α_v/c_v (10^3 J)**
SrS	12.2	14.51	694.32	1.85	6.42
SrSe	8.29	8.9	430.38	3.16	9.80
SrTe	1.20	3.05	146.16	2.30	6.23

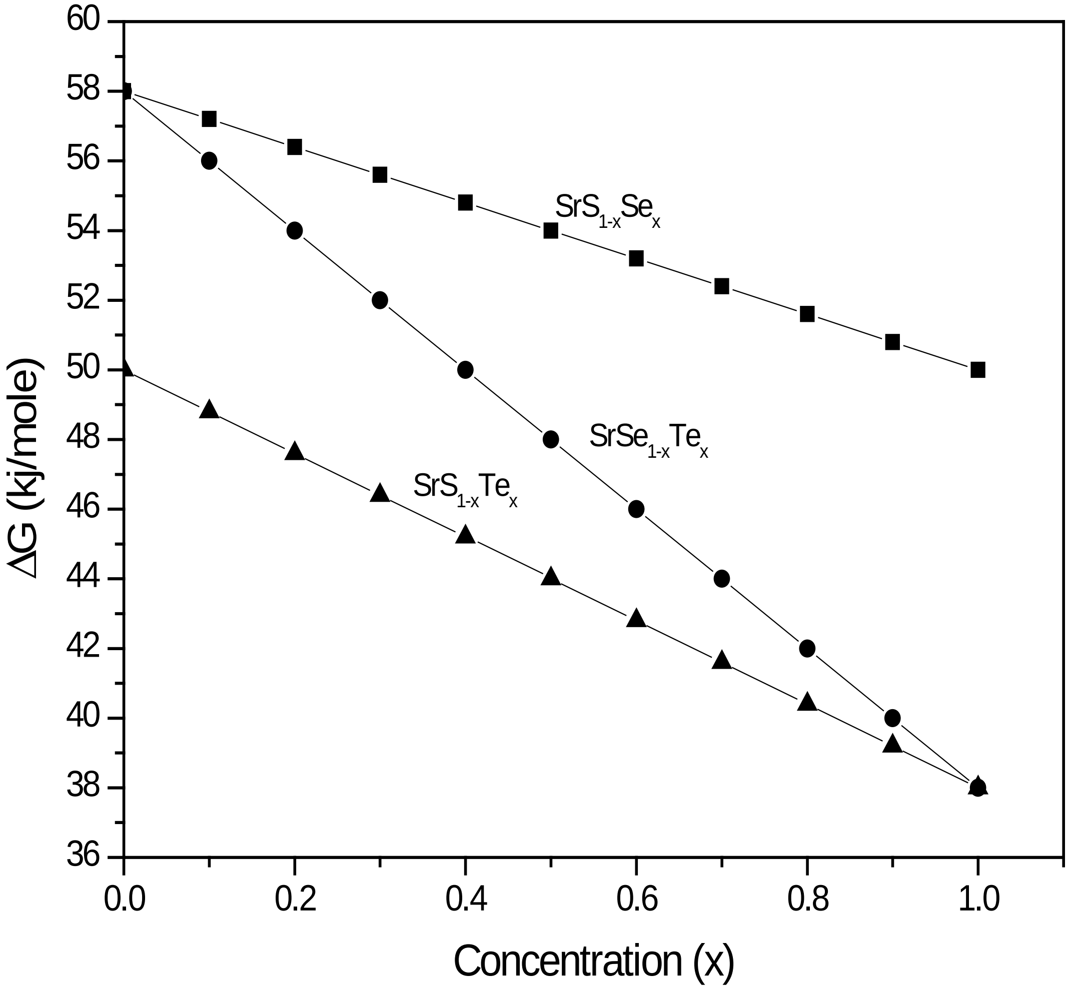

Fig 1.

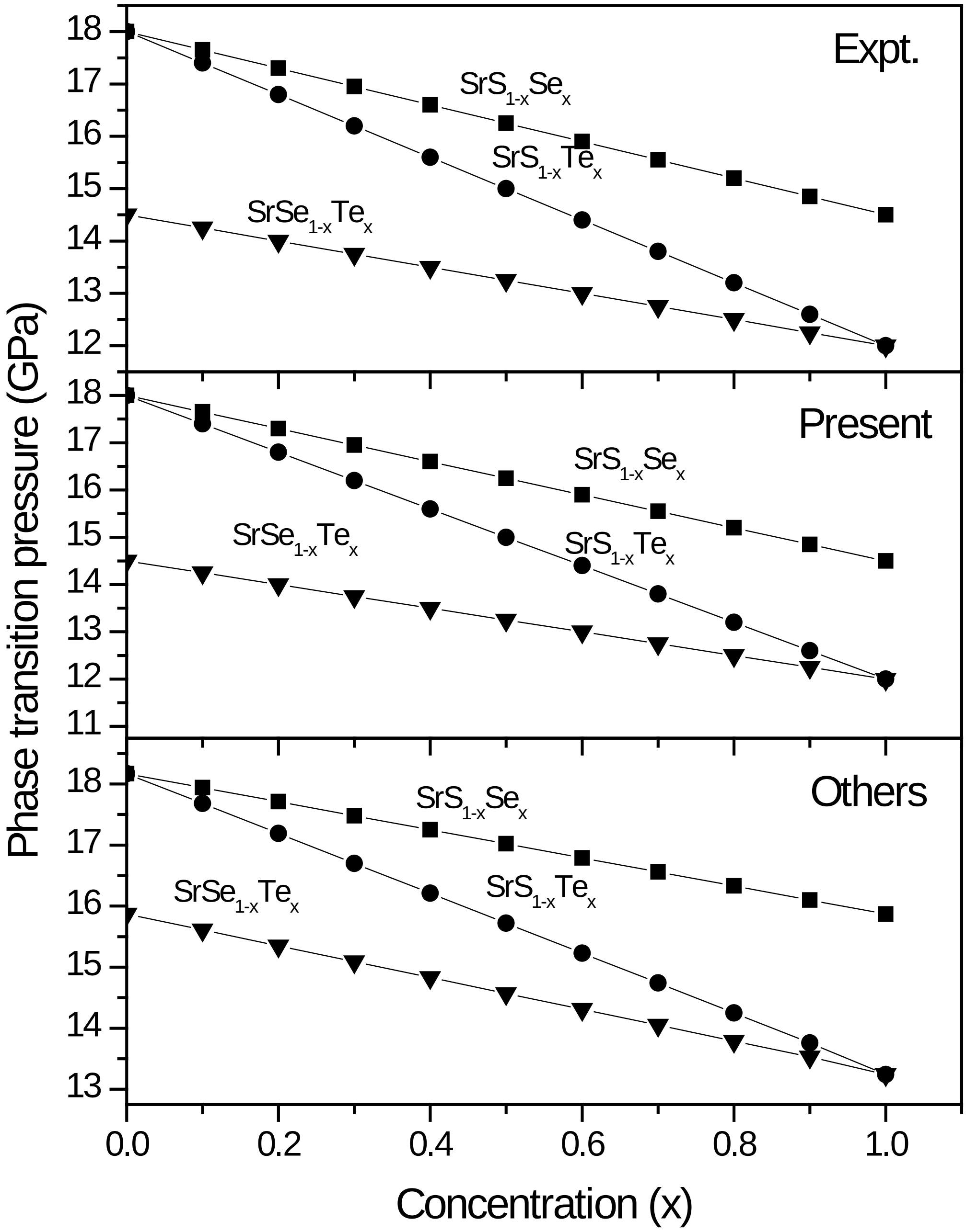
Expt.
Present
Others
$SrS_{1-x}Se_x$
$SrS_{1-x}Te_x$
$SrSe_{1-x}Te_x$
Phase transition pressure (GPa)
Concentration (x)
18
17
16
15
14
13
12
11
0.0
0.2
0.4
0.6
0.8
1.0

Fig 2.

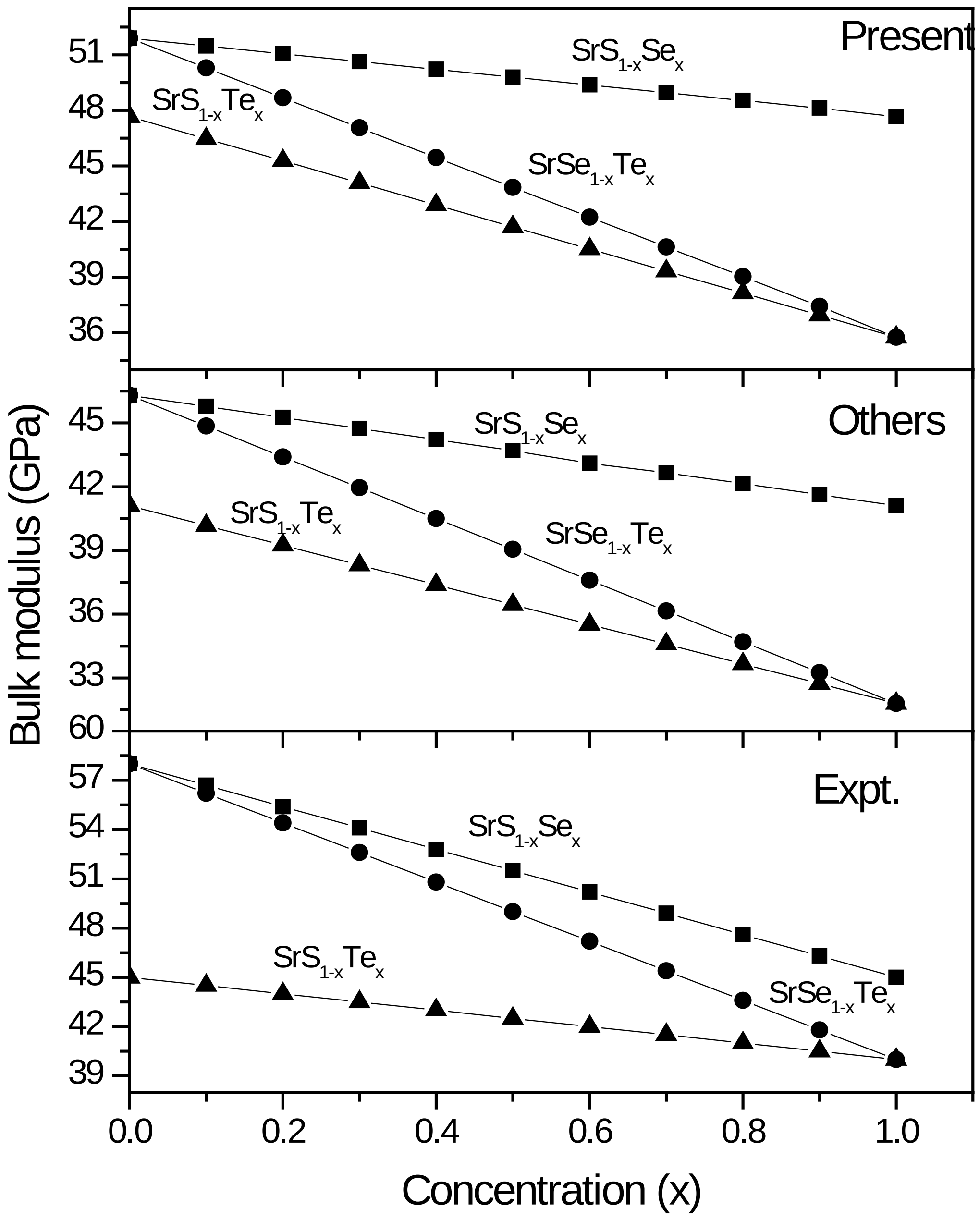
Present
Others
Expt.
SrS1-xSex
SrS1-xTex
SrSe1-xTex
Bulk modulus (GPa)
Concentration (x)
51
48
45
42
39
36
33
60
57
54
0.0
0.2
0.4
0.6
0.8
1.0

Fig 3.