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Elastic and lattice dynamical properties of ternary strontium chalcogenide alloys

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ABSTRACT

The structural and elastic properties, and lattice dynamics of the ternary alloys $SrS_{1-x}Se_x$, $SrS_{1-x}Te_x$ and $SrSe_{1-x}Te_x$ have been studied using first principles calculations. The density functional perturbation theory (DFPT) and the virtual crystal approximation (VCA) are employed. The variation of the structural parameters, the elastic constants, the optical and acoustic phonon frequencies at the high symmetry points Γ, X and L, the electronic and static dielectric constants, the Born effective charge are studied as a function of the concentration (x). All these properties follow a quadratic law in x and the values of the bowing parameters for $SrS_{1-x}Te_x$ are larger than for the other two alloys. The structural and elastic properties for simple cubic supercells with x=0.25, 0.5, and 0.75 have been computed and they are in good agreement with those obtained from VCA.

1. Introduction

The strontium chalcogenides SrS, SrSe and SrTe are of great technological interest with many application ranging from catalysis to microelectronics. They have applications in the area of luminescent devices and infrared sensitive devices [1–3]. These compounds form a closed shell ionic system crystallizing in the NaCl structure at normal conditions, undergo a pressure induced first order structural phase transition to CsCl-type (B2) structure [4–6].

There are a number of reported works on these materials concerning electronic band structure, volume dependence of energy gap, optical properties, structural phase stability, elastic properties, lattice dynamics, thermodynamic properties and metallization process [7–29].

However, the properties of the ternary $SrS_{1-x}Se_x$, $SrS_{1-x}Te_x$ and $SrSe_{1-x}Te_x$ alloys are less studied. We notice the two theoretical works of Labidi et al. [30,31], using the linearized augmented plane wave method to investigate the structural, optical and electronic properties of these alloys. Recently, Bhardwaj [32] used a newly developed three body potential including covalency effect to study the phase transition, the mechanical and the thermal properties of the above cited alloys in which the predicted bulk modulus values vary linearly with concentration. To the best of our knowledge, there are no reported theoretical nor experimental studies on the elastic and vibrational properties of these alloys.

The aim of this work is to present first principles calculations of the structural, elastic properties and lattice dynamics of $SrS_{1-x}Se_x$, $SrS_{1-x}Te_x$ and $SrSe_{1-x}Te_x$ as a function of the composition (x) in the rocksalt phase. We study the variation of the lattice parameter, bulk modulus, elastic constants (c_{11}, c_{12} and c_{44}), the phonon frequencies at high symmetry points Γ, X and L, electronic and static dielectric constants ($\epsilon_\infty, \epsilon(0)$) and the Born effective charge (Z^*) with the composition (x). The calculations are performed using the plane wave pseudopotentail method within the density functional theory and the linear response technique using the virtual crystal approximation

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Table 1
Calculated lattice parameter a_0 in (Å), Bulk modulus B in (GPa) for $SrS_{1-x}Se_x$, $SrS_{1-x}Te_x$ and $SrSe_{1-x}Te_x$. The values between parenthesis are the LDA ones.

	x	Lattice constant, a_0			Bulk modulus, B (GPa)		
Alloy		Present	Exp.	Others	Present	Exp.	Others
$SrS_{1-x}Se_x$	0	6.05[a] (5.90)	6.024[b]	6.065[c], 5.90[d], 5.77[g]	48.30[a] (57.68)	58[b]	46.3[c], 57.7[d], 62[g], 51[h]
VCA	0.25	6.127 (5.968)			45.477 (54.834)		
SC		6.118 (5.958)		6.133[c], 5.962[d]	45.786 (55.050)		45.6[c], 55.7[d], 50.84[h]
VCA	0.50	6.191 (6.026)			43.499 (52.586)		
SC		6.180 (6.014)		6.195[c], 6.018[d]	43.901 (52.923)		44.8[c], 53.6[d], 49.78[h]
VCA	0.75	6.247 (6.077)			41.985 (50.802)		
SC		6.239 (6.068)		6.251[c], 6.071[d]	42.234 (50.988)		43.5[c], 51.5[d], 48.72[h]
	1	6.29[a] (6.12)	6.23[e]	6.30[c], 6.12[d], 6.02[g]	40.93[a] (49.39)	45[e]	41.1[c], 49.8[d], 52[g], 47.66[h]
$SrS_{1-x}Te_x$	0	6.05[a] (5.90)	6.024[b]	6.065[c], 5.90[d], 5.77[g]	48.30[a] (57.68)	58[b]	46.3[c], 57.7[d], 62[g], 51.9[h]
VCA	0.25	6.300 (6.136)			40.507 (48.660)		
SC		6.252 (6.084)		6.267[c]	41.946 (50.398)		41.6[c], 47.87[h]
VCA	0.50	6.481 (6.307)			36.286 (43.772)		
SC		6.426 (6.248)		6.417[c]	37.703 (45.416)		37.5[c], 43.84[h]
VCa	0.75	6.616 (6.430)			33.745 (40.768)		
SC		6.581 (6.395)		6.596[c]	34.50 (41.671)		33.5[c], 39.81[h]
	1	6.71[a] (6.52)	6.66[f]	6.735[c], 6.48[g]	32.07[a] (38.92)	39.5[f]	31.8[c], 44[g], 35.76[h]
$SrSe_{1-x}Te_x$	0	6.29[a] (6.12)	6.23[e]	6.30[c], 6.12[d], 6.02[g]	40.93[a] (49.39)	45[e]	41.1[c], 49.8[d], 52[g], 47.66[h]
VCA	0.25	6.432 (6.252)			37.547 (45.257)		
SC		6.415 (6.199)		6.412[c]	37.862 (45.769)		38.1[c], 44.69[h]
VCA	0.50	6.545 (6.361)			35.132 (42.428)		
SC		6.525 (6.339)		6.525[c]	33.304 (40.351)		34.0[c], 41.72[h]
VCA	0.75	6.673 (6.45)			32.699 (42.985)		
SC		6.626 (6.435)		6.641[c]	33.605 (40.696)		32.0[c], 38.75[h]
	1	6.71[a] (6.52)	6.66[f]	6.735[c], 6.48[g]	32.07[a] (38.92)	39.5[f]	31.8[c], 44[g], 35.76[h]

[a] Ref. [29]. PP–PW+GGA.
[b] Experimental data of Ref. [4].
[c] Ref. [30]. FP–LAPW+GGA.
[d] Ref. [31]. FP–LAPW+LDA.
[e] Experimental data of Ref. [5].
[f] Experimental data of Ref. [6].
[g] Ref. [24]. TB–LMTO+LDA.
[h] Ref. [32]. Three body potential model.

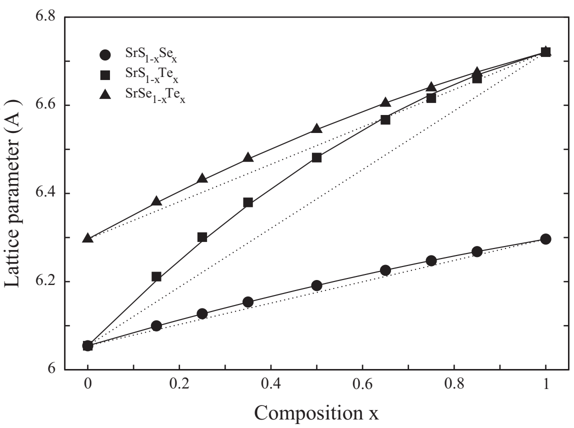

Fig. 1. Composition dependence of the calculated lattice constant using the VCA. Solid line is the quadratic fit to our data and the dashed line represents Vegard's law.

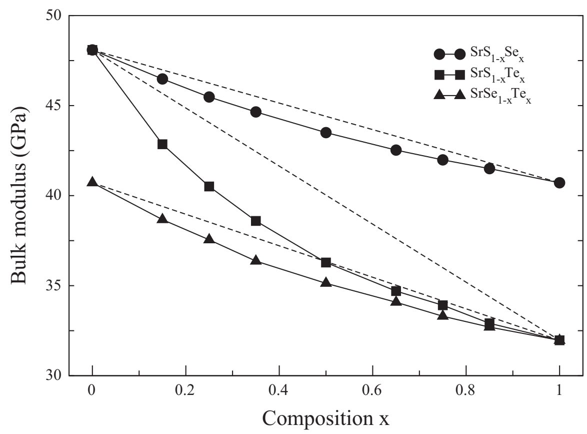

Fig. 2. Composition dependence of the calculated bulk modulus using the VCA. Dashed line is the LCD prediction.

(VCA), which is known to be a simple and efficient one [33]. It has been successfully used in many systems [34–43]. We have also calculated the structural properties and elastic constants tensors for simple cubic 8-atom supercells (SCs) [44], containing 1 (x=0.25), 2 (x=0.50) and 3 (x=0.75) substitutional Se (Te) atoms on the S (Se) sites in order to compare with those obtained from VCA method.

In our calculation, we have used both the local density approximation (LDA) and the generalized gradient approximation (GGA). We have found that for the binaries for