

Non – linear properties of mixed divalent crystals

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ABSTRACT

Rare-earth alloys with the IV-VI compounds semiconductors have been extensively studied in recent years because of their scientific and technology interest. One possible application for alloys of rare-earth elements with lead salts therefore resides in the emerging field of spintronics. Lead selenide is an important semiconductor which finds application in several devices including IR radiation and photoconductor detector as well as photovoltaic material. Solid solutions based on lead chalcogenides have been used as efficient materials for long wave lasers and also in the construction of infrared detectors for the 8-14 μm atmospheric windows. The knowledge of the non-linear properties plays an important part in providing valuable information about the mechanical and dynamical properties, such as inter atomic potentials, equation of state, and phonon spectra. Elastic properties are also thermodynamically related to the specific heat, thermal expansion, Debye temperature, melting point and Grüneisen parameter. The elastic constants are believed to be related to the strength of materials. Indeed, the latter has been often related to the bulk modulus, shear modulus, young's modulus, and poisson's ratio, which are frequently measured for polycrystalline materials when investigating their hardness. The aim of this work is to give a detailed description of the behavior of non-linear properties such as second, third and fourth order elastic constants of $(\text{PbSe})_x - (\text{PbTe})_{1-x}$ at an elevated temperature starting from 50K up to 1200K by using Coulomb and Börn - Mayer potentials. The evaluation of other non-linear properties such as first order pressure derivatives of second and third order elastic constants, second order pressure derivatives of second order elastic constants and partial contractions are computed using higher order elastic constants using this theory.

INTRODUCTION

Great quantities of Lead, both as the dioxide and the metal, are used in batteries, cable covering, plumbing, and ammunition. Lead chalcogenides are important materials for applications such as IR detectors, photographic plates, and photo resistors. These materials exhibit low thermal conductivity which is closely related to their lattice dynamics and thermodynamic properties. Among the group IV-VI compounds, Lead selenide thin film is used as a target material in infrared sensor, grating, lenses and various optoelectronic devices. It has a higher thickness and a direct band gap of 0.27 eV in room temperature. Lead telluride, lead antimonide and lead selenide are some of the lead based semiconductors which are used in photovoltaic cells and infrared detectors. Lead selenide nano-crystals embedded into various materials can be used as quantum dots. Lead Telluride is used in a number of industrial applications including infrared detection and imaging. Resonant ultrasound spectroscopy was utilized to determine the temperature dependence of elastic moduli, including Young's modulus, shear modulus and Poisson's ratio of Lead telluride based thermo elastic materials. PbTe single crystals doped with VII A Periodic system group elements will continue to attract a widespread attention both for their fundamental electronic properties and for the applications in infrared optoelectronic [1-3]. Studies on mixed crystals are quite useful as they are of considerable technological importance in the field of storage cells. Elasticity of crystalline solid is, like other physical properties, strongly anisotropic and is conveniently represented by tensor elastic constants. Ultrasonic characterization of materials is a versatile tool for the inspection of their micro-structure and their mechanical properties. This is possible because of the close association of the ultrasound wave with the elastic and the inelastic properties of the materials; also this technique offers the possibility of using different frequency ranges and many modes of vibration of the ultrasound waves to probe into structural level [4].

An investigation in to the higher order elastic constants and their pressure derivatives provides useful information on the interatomic forces and on anharmonic properties of crystalline solids. The elasticity relates to forces acting between atoms or ions in crystals, or the interatomic potentials. Static and dynamic properties of crystal lattices are treated by the theory of lattice dynamics; they can also be treated by the theory on the basis of the long-wave or continuum approximation. The approximation is acceptable when spatial variation of atomic displacement is small compared with inter-atomic spacing. The elasticity theory is convenient because the number of elastic constants required to describe crystal properties is smaller than the number of force constants in lattice dynamical theory, and the elastic constants of common crystals can be determined accurately by simple experiments. The temperature dependence of the elastic constants in pure perfect crystals, dielectrics, and semiconductors is determined by the anharmonicities of the vibrations of the crystal lattice [5-8]. The elastic constants are strongly related to other anharmonic properties and used to evaluate thermo elastic constants, thermal conductivity, elastic properties [9-12], ultrasonic parameters such as ultrasonic velocities, thermal expansion, thermal relaxation time etc. Elastic properties of solid are important because they are closely related to various fundamental solid state phenomena such as interatomic bonding, equation of state and phonon spectra. Most important knowledge of elastic constants is essential for many particle applications related to the mechanical

properties of solids; load deflection, thermo elastic stress, internal strain and fracture toughness. The variation of elastic constants [13, 14] with respect to pressure can reveal many important features of the short range forces at high pressure. If the value of second order elastic constants and density at a particular temperature are known for any crystalline solid, one may obtain ultrasonic velocity for longitudinal and shear waves which give an important information about its internal structure, inherent and anharmonic properties. It is also known that the third order elastic constants govern a number of non-linear acoustical properties of a solid, such as the distortion of the acoustic waveform or the generation of higher harmonics, the possibility of combination scattering of sound by sound. Higher order elastic constants are important in the calculation of many anharmonic effects, such as temperature dependence of the second order elastic constants and thermal expansion. In addition, one may be able to assess the relative importance of different contributions to the interaction energy between atoms in crystals from these constants. The ultrasonic studies [15] can provide interesting information on the specificities of ion-solvent interaction related to the structure of the solute and the reciprocal effects which arise in the solvent. There are only few studies on the behavior of the elastic constants in comparison to the existing number of studies on the behavior of long wavelength crystal vibration in mixed crystals [16, 17]. One has developed a theory which starts from nearest neighbor distance and hardness parameter of crystal using Coulomb and Born-Mayer potentials for obtaining various non – linear properties at different temperature for mixed crystals. The long wave length response of a solid to a theoretical model forms the basis of lattice dynamical studies in as much as the model parameters are fixed by this response. Thus second order elastic constants related with the long wave length acoustical model and long wave length optical vibration frequencies are the basic input data in most lattice dynamical studies on ionic solids. The applicability of a model to a system of solids largely depends on whether the model is capable of giving a good description of these input parameters. From this view point Coulomb and Born-Mayer models are possibly ideal for ionic crystals [18, 19].

To evaluate the non-linear properties for a deformed crystal, the elastic energy density is expanded by Taylor's series expansions. One gets a series with higher order coefficients. These coefficients are known as higher order elastic constants. In this expansion, the second, third and fourth order elastic constants are the coefficients of second, third and fourth order terms. When the values of these elastic constants of substance are known, many of the anharmonic properties of the substances can be treated within the limit of the continuum approximation in a quantitative manner. In last and present decade considerable interest has been taken in investigation of ultrasonic properties of materials [20-23]. Elastic and dielectric properties of mixed ionic solids have been carried out by number of workers using different phenomenological models. The present theory deals with temperature dependence of elastic properties of mixed (PbSe)_x - (PbTe)_{1-x} crystals having face centered cubic crystal symmetry. In present investigation, some efforts have been made for obtaining SOECs, TOECs and FOECs at an elevated temperature, the FOPDs of SOECs and TOECs, the SOPDs of SOECs and partial contractions of mixed (PbSe)_x - (PbTe)_{1-x} crystals.

FORMULATION

As we presented earlier the elastic energy density for a crystal of a cubic symmetry can be expanded up to quartic terms as shown below [24];

$$U_0 = U_2 + U_3 + U_4$$

$$= [1/2!]C_{ijkl} X_{ij} X_{kl} + [1/3!]C_{ijklmn} X_{ij} X_{kl} X_{mn} + [1/4!]C_{ijklmpq} X_{ij} X_{kl} X_{mn} X_{pq} \quad (1)$$

Where C_{ijkl} , C_{ijklmn} and $C_{ijklmpq}$ are the SOECs, TOECs and FOECs in tensorial form; e_{ij} are the Lagrangian strain components. The SOECs, TOECs and FOECs are as given below:

$$C_{ijkl} = C_{IJ} = (\partial^2 U / \partial e_{ab} \partial e_{cd})_{\epsilon=0}, \quad C_{ijklmn} = C_{IJK} = (\partial^3 U / \partial e_{ab} \partial e_{cd} \partial e_{mn})_{\epsilon=0}$$

$$\text{and} \quad C_{ijklmpq} = C_{IJKL} = (\partial^4 U / \partial e_{ab} \partial e_{cd} \partial e_{mn} \partial e_{pq})_{\epsilon=0} \quad (2)$$

Where C_{IJ} , C_{IJK} and C_{IJKL} are the second, third and fourth order elastic constants in Brügger's definition and Voigt notations. These elastic constants have two parts as given below [25, 26];

$$C_{IJ} = C_{IJ}^0 + C_{IJ}^{vib}, \quad C_{IJK} = C_{IJK}^0 + C_{IJK}^{vib}, \quad C_{IJKL} = C_{IJKL}^0 + C_{IJKL}^{vib} \quad (3)$$

EVALUATION

When a cubic crystal is subjected to hydrostatic pressure, the symmetry of the crystal is preserved. It is well known that the contribution of the FOECs to a number of anharmonic effects like thermal expansion, pressure derivatives of the TOECs, the temperature dependence of the SOECs etc., may be comparable to that arising from the TOECs. The inclusion of the fourth order strain components in the strain energy expression should be necessary in a study of the effect of large stresses on elastic solids [27]. With the help of nearest-neighbour distance and hardness parameter; the second, third and fourth order elastic constants for mixed (PbSe)_x - (PbTe)_{1-x} crystals are evaluated at different temperature (from 50K to up to 1150K). The values of the second, third and fourth order elastic constants at 300K for mixed (PbSe)_x - (PbTe)_{1-x} crystals are given in Tables 1 – 3. The FOPDs of SOECs and TOECs, the SOPDs of SOECs and partial contractions for this material are evaluated utilizing room temperature, and the results are shown in Tables 4 – 5.

RESULT AND DISCUSSION

The study of mixed crystal is useful in many technological applications. There has been considerable interest in the physical properties of mixed crystals as they find interesting applications and their study helps in understanding basic mechanism of mixed crystal formation. The variation of activation energies in mixed crystals is correlated to lattice distortion and an increase of trivalent ion concentration. A mixed crystal has physical properties analogous to those of the pure crystals. The composition dependence varies from system to system and from property to property [28-30]. The SOECs, TOECs and FOECs in 10^{10} N/m² at room temperature for mixed (PbSe)_x - (PbTe)_{1-x} crystals are shown in Tables 1 – 3. The FOPDs of the SOECs and TOECs of mixed (PbSe)_x - (PbTe)_{1-x} are presented in Table 4. The SOPDs of the SOECs in 10^{-11} m²/N and partial contractions in 10^{12} N/m² are shown in Table 5.

The temperature variation of various anharmonic properties such as temperature variation of SOECs, TOECs and FOECs, FOPDs of SOECs and TOECs, the SOPDs of SOECs and partial contractions are represented graphically for mixed (PbSe)_x - (PbTe)_{1-x}. Many useful properties of solid state materials are related with their anharmonic behavior. For cubic crystals there are three independent second order elastic constants. We can say from Table 1, all the data of SOECs are positive in nature. The values of C_{11} and C_{44} are increasing and the value of C_{12} is decreasing as temperature increases for mixed (PbSe)_x - (PbTe)_{1-x} crystals. It is clear from Figure 1; the value of C_{11} and C_{44} are increasing and the value of C_{12} is decreasing as temperature increases for mixed (PbSe)₁₀₀ - (PbTe)₀ crystals. The TOECs of materials provide extremely important information, concerning their anharmonic behaviour and have therefore been the subject of a number of theoretical and experimental studies. There are six third order elastic constants for mixed (PbSe)_x - (PbTe)_{1-x} at 300K. For all mixed crystals the values of C_{111} , C_{112} and C_{166} are negative in nature while C_{123} , C_{144} and C_{456} are positive in nature. Temperature variation of third order elastic constants shown that the values of C_{111} , C_{123} , C_{144} and C_{166} are increasing; the value of C_{112} is decreasing as temperature increases and C_{456} remains constant for all mixed lead selenide and telluride crystals. For mixed (PbSe)₈₀ - (PbTe)₂₀; the values of C_{111} , C_{123} , C_{144} and C_{166} are increasing and the value of C_{112} is decreasing as temperature increases while C_{456} remains constant shown in Figures 2(i) and 2(ii).

Higher order elastic constants are important for the study of the anharmonic behaviour of solids. The fourth order elastic constants can be obtained as function of the derivatives of sound velocities with respect to applied pressure or uniaxial stress, which in turn can be directly derived from the crystal potentials. There are eleven fourth order elastic constants for divalent crystals. For all mixed (PbSe)_x - (PbTe)_{1-x} crystals, the values of C_{1111} , C_{1112} , C_{1122} , C_{1144} , C_{1155} , C_{1255} , C_{1266} , C_{4444} and C_{4455} is decreasing as temperature increases and the value of C_{1123} is increasing as temperature increases. The value of C_{1456} remains constant. Figures [3(i)–3(iv)] shown the temperature variation of fourth order elastic constants for mixed (PbSe)₆₀ - (PbTe)₄₀. There are three FOPDs of SOECs and six of TOECs for mixed crystals. Figure 4 present the temperature variation of FOPDs of SOECs for mixed (PbSe)₀ - (PbTe)₁₀₀. From this figure, it is clear that the value of dC_{11}/dp and dC_{12}/dp decreases and the value of dC_{44}/dp first increases from temperature 50K to 200K and constant from 200K to 500 K than decreases as temperature increases. For all mixed crystals the values of dC_{111}/dp , dC_{112}/dp , dC_{144}/dp , dC_{166}/dp and dC_{456}/dp are increases and the value of dC_{123}/dp decreases as temperature increases. Figures 5(i) and 5(ii) shows that the values of dC_{111}/dp , dC_{112}/dp , dC_{144}/dp , dC_{166}/dp and dC_{456}/dp are increases and the value of dC_{123}/dp decreases as temperature increases for mixed (PbSe)₄₀ - (PbTe)₆₀. There are three second order pressure derivatives of second order elastic constants for all mixed crystals. It may be stated that all the SOPDs of SOECs are positive. Figure 6 present the value of d^2C_{11}/dp , and d^2C_{44}/dp decreases as temperature increases and d^2C_{12}/dp first decreases than increases as temperature increases for mixed (PbSe)₈₀ - (PbTe)₂₀. There are three partial contractions for mixed lead selenide and telluride crystals at 300K. The values of partial contractions for all fractions of mixed lead selenide and telluride crystals are decreasing. From Figure 7, one can say that the value of Ψ_{11} , Ψ_{12} and Ψ_{44} decreases as temperature increases for mixed (PbSe)₄₀ - (PbTe)₆₀. The data obtained in present investigation will be helpful to those workers who are engaged in such studies.

ACKNOWLEDGEMENT

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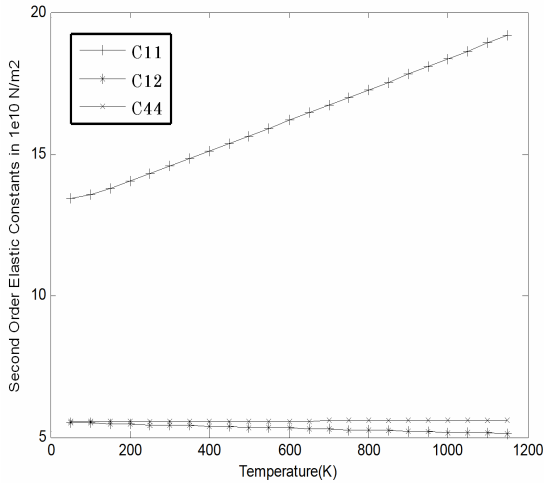


Figure 1. Temperature Variation of SOECs for mixed $(\text{PbSe})_{100} - (\text{PbTe})_0$

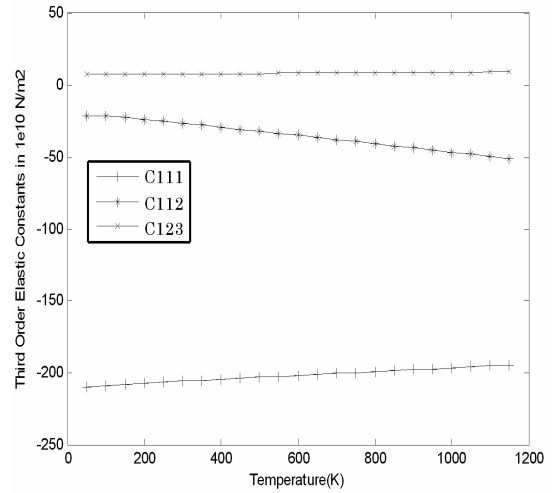


Figure 2(i). Temperature Variation of TOECs for mixed $(\text{PbSe})_{80} - (\text{PbTe})_{20}$

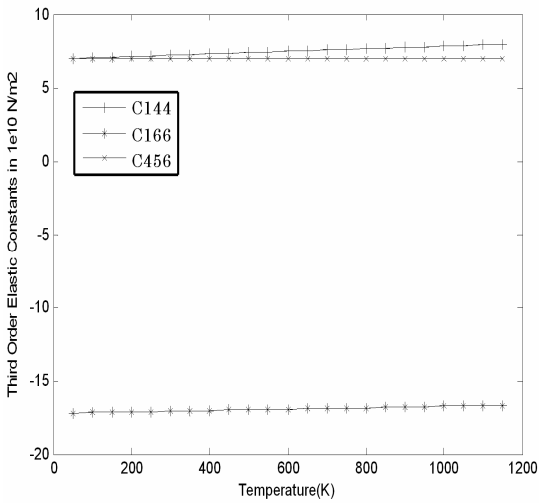


Figure 2(ii). Temperature Variation of TOECs for mixed $(\text{PbSe})_{80} - (\text{PbTe})_{20}$

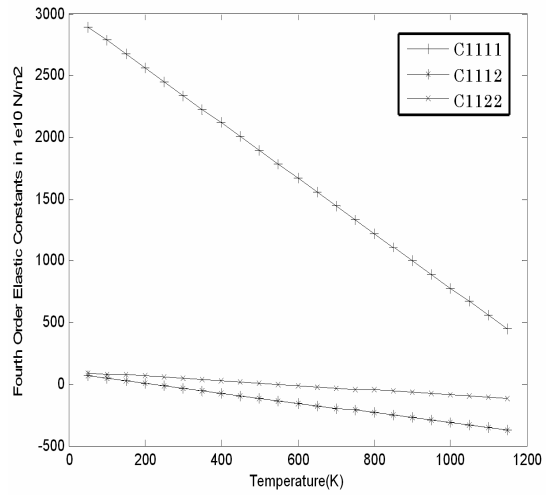


Figure 3(i). Temperature Variation of FOECs for mixed $(\text{PbSe})_{60} - (\text{PbTe})_{40}$

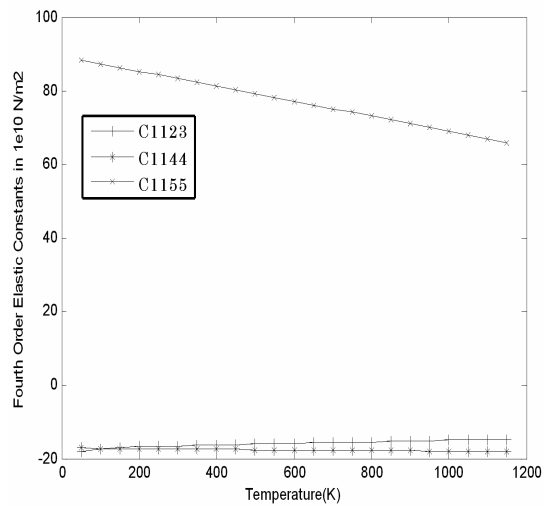


Figure 3(ii). Temperature Variation of FOECs for mixed $(\text{PbSe})_{60} - (\text{PbTe})_{40}$

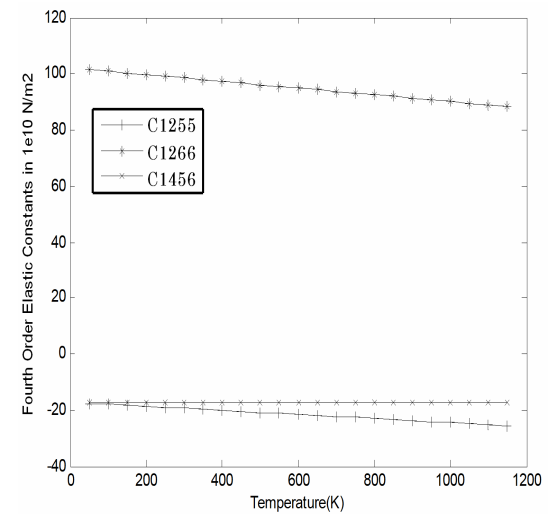


Figure 3(iii). Temperature Variation of FOECs for mixed $(\text{PbSe})_{60} - (\text{PbTe})_{40}$

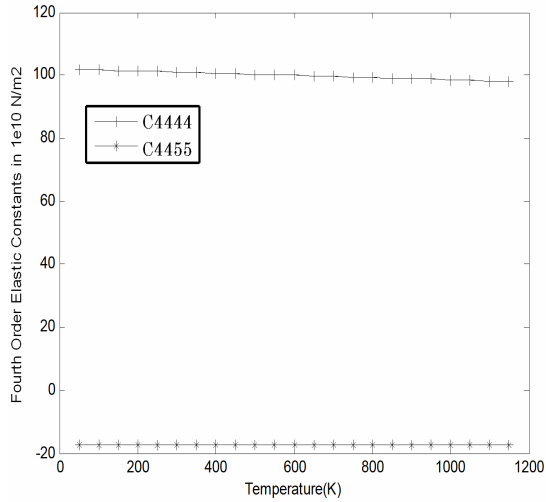


Figure 3(iv). Temperature Variation of FOECs for mixed (PbSe)₆₀–(PbTe)₄₀

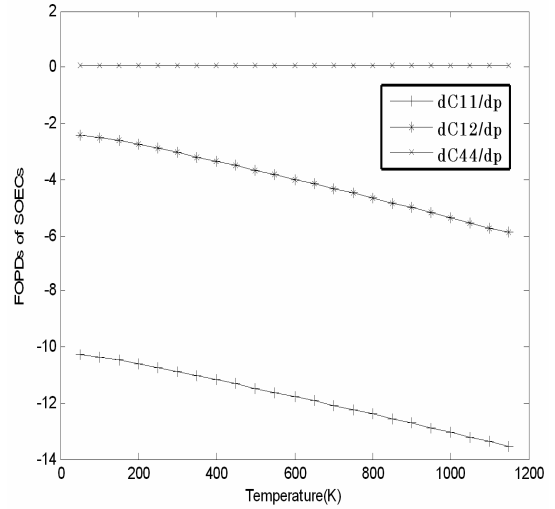


Figure 4. Temperature Variation of FOPDs for mixed (PbSe)₀–(PbTe)₁₀₀

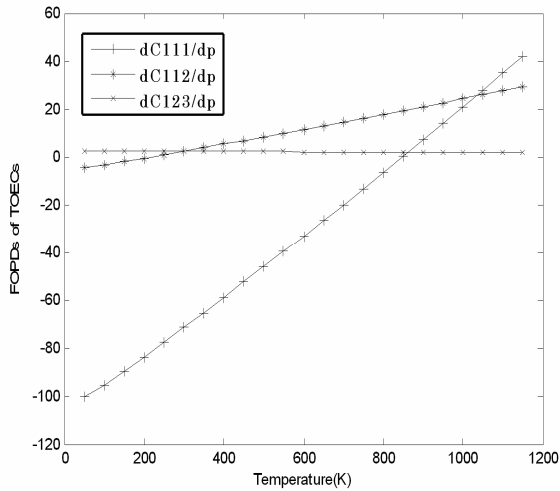


Figure 5(i). Temperature Variation of FOPDs for mixed (PbSe)₄₀–(PbTe)₆₀

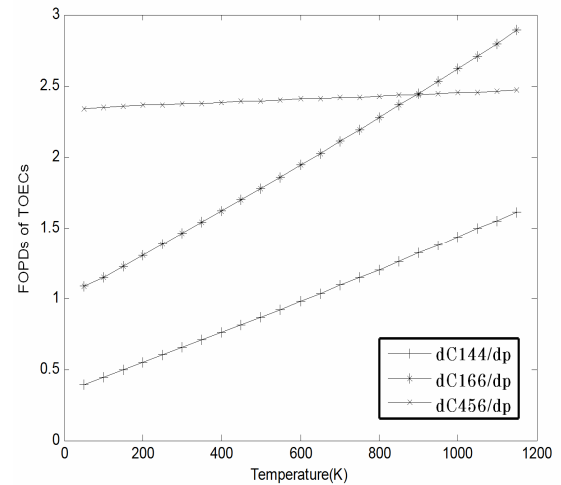


Figure 5(ii). Temperature Variation of FOPDs for mixed (PbSe)₄₀–(PbTe)₆₀

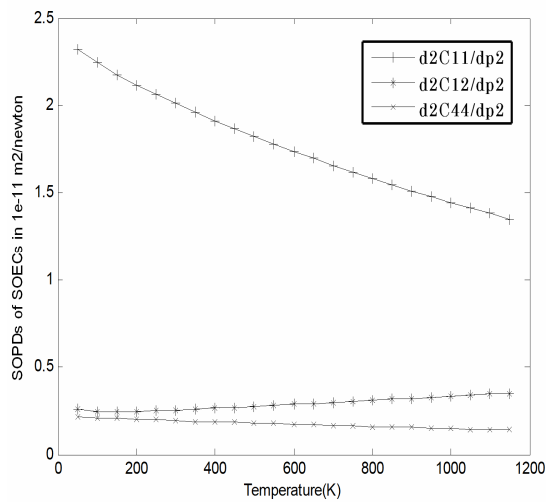


Figure 6. Temperature Variation of SOPDs for mixed (PbSe)₈₀–(PbTe)₂₀

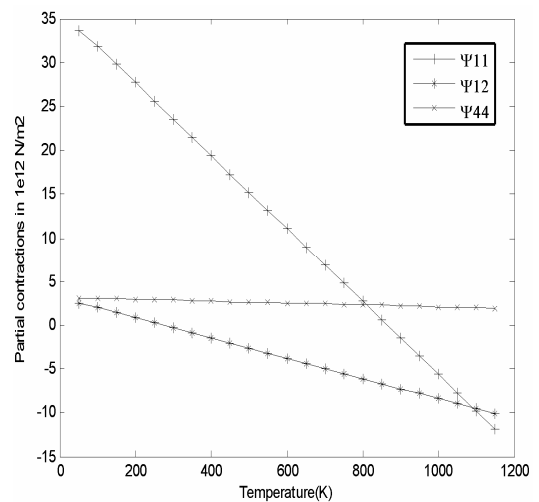


Figure 7. Temperature Variation of Partial Contractions for mixed (PbSe)₄₀–(PbTe)₆₀

Table 1. Second Order Elastic Constants in 10^{10} N/m² at room temperature for mixed (PbSe)_x - (PbTe)_{1-x}

Fraction	(PbSe) ₁₀₀ - (PbTe) ₀	(PbSe) ₈₀ - (PbTe) ₂₀	(PbSe) ₆₀ - (PbTe) ₄₀	(PbSe) ₄₀ - (PbTe) ₆₀	(PbSe) ₂₀ - (PbTe) ₈₀	(PbSe) ₀ - (PbTe) ₁₀₀
C ₁₁	14.576	14.665	15.024	15.389	15.762	13.043
C ₁₂	5.418	4.109	4.375	4.664	4.976	3.938
C ₄₄	5.545	4.233	4.502	4.794	5.109	4.052

Table 2. Third Order Elastic Constants in 10^{10} N/m² at room temperature for mixed (PbSe)_x - (PbTe)_{1-x}

Fraction	(PbSe) ₁₀₀ - (PbTe) ₀	(PbSe) ₈₀ - (PbTe) ₂₀	(PbSe) ₆₀ - (PbTe) ₄₀	(PbSe) ₄₀ - (PbTe) ₆₀	(PbSe) ₂₀ - (PbTe) ₈₀	(PbSe) ₀ - (PbTe) ₁₀₀
C ₁₁₁	-220.850	-206.110	-209.799	-213.498	-217.186	-202.423
C ₁₁₂	-31.767	-26.537	-27.688	-28.937	-30.293	-25.470
C ₁₂₃	9.425	7.459	7.900	8.373	8.881	7.046
C ₁₄₄	9.048	7.200	7.613	8.500	8.535	6.813
C ₁₆₆	-22.081	-17.087	18.195	-19.392	-20.685	-16.057
C ₄₅₆	8.723	6.934	7.334	7.764	8.226	6.560

Table 3. Fourth Order Elastic Constants in 10^{10} N/m² at room temperature for mixed (PbSe)_x - (PbTe)_{1-x}

Fraction	(PbSe) ₁₀₀ - (PbTe) ₀	(PbSe) ₈₀ - (PbTe) ₂₀	(PbSe) ₆₀ - (PbTe) ₄₀	(PbSe) ₄₀ - (PbTe) ₆₀	(PbSe) ₂₀ - (PbTe) ₈₀	(PbSe) ₀ - (PbTe) ₁₀₀
C ₁₁₁₁	2457.17	2304.64	2343.89	2382.56	2420.38	2264.77
C ₁₁₁₂	-10.12	-38.22	-31.75	-24.98	-17.78	-44.16
C ₁₁₂₂	71.12	37.80	45.39	53.47	62.03	30.59
C ₁₁₂₃	-20.02	-15.53	-16.53	-17.61	-18.77	-14.59
C ₁₁₄₄	-20.67	-16.44	-17.39	-18.40	-19.49	-15.56
C ₁₁₅₅	101.05	78.11	83.22	88.73	94.66	73.34
C ₁₂₅₅	-22.90	-18.33	-19.36	-20.46	-21.64	-17.37
C ₁₂₆₆	119.03	92.63	98.52	104.87	111.69	87.13
C ₁₄₅₆	-20.38	-16.20	-17.14	-18.14	-19.22	-15.33
C ₄₄₄₄	121.83	95.03	101.02	107.47	114.39	89.44
C ₄₄₅₅	-20.47	-16.27	-17.20	-18.22	-19.30	-15.39

Table 4. First Order Pressure Derivatives of the Second and Third Order Elastic Constants for $(\text{PbSe})_x - (\text{PbTe})_{1-x}$

Fraction	$(\text{PbSe})_{100} - (\text{PbTe})_0$	$(\text{PbSe})_{80} - (\text{PbTe})_{20}$	$(\text{PbSe})_{60} - (\text{PbTe})_{40}$	$(\text{PbSe})_{40} - (\text{PbTe})_{60}$	$(\text{PbSe})_{20} - (\text{PbTe})_{80}$	$(\text{PbSe})_0 - (\text{PbTe})_{100}$
dC_{11} / dp	-9.861	-10.687	-10.482	-10.275	-10.068	-10.893
dC_{12} / dp	-3.018	-3.031	-3.024	-3.019	-3.017	-3.040
dC_{44} / dp	0.201	0.087	0.114	0.142	0.171	0.061
dC_{111} / dp	-68.845	-73.956	-72.779	-71.532	-70.221	-75.068
dC_{112} / dp	1.200	3.563	2.945	2.344	1.763	4.202
dC_{123} / dp	2.287	2.157	2.189	2.221	2.253	2.127
dC_{144} / dp	0.693	0.610	0.630	0.651	0.672	0.590
dC_{166} / dp	1.446	1.469	1.463	1.457	1.451	1.476
dC_{456} / dp	2.416	2.329	2.350	2.371	2.393	2.309

Table 5. SOPDs of the SOECs in $10^{-11} (\text{N/m}^2)^{-1}$ and Partial Contraction (Ψ in 10^{12}N/m^2) for $(\text{PbSe})_x - (\text{PbTe})_{1-x}$

Fraction	$(\text{PbSe})_{100} - (\text{PbTe})_0$	$(\text{PbSe})_{80} - (\text{PbTe})_{20}$	$(\text{PbSe})_{60} - (\text{PbTe})_{40}$	$(\text{PbSe})_{40} - (\text{PbTe})_{60}$	$(\text{PbSe})_{20} - (\text{PbTe})_{80}$	$(\text{PbSe})_0 - (\text{PbTe})_{100}$
$d^2 C_{11} / dp^2$	1.571	2.011	1.893	1.781	1.673	2.134
$d^2 C_{12} / dp^2$	0.224	0.254	0.246	0.238	0.231	0.263
$d^2 C_{44} / dp^2$	0.179	0.194	0.190	0.186	0.183	0.198
Ψ_{11}	25.189	21.967	22.746	23.544	24.358	21.201
Ψ_{12}	0.219	-0.783	-0.554	-0.311	-0.054	-1.001
Ψ_{44}	3.254	2.495	2.664	2.846	3.042	2.338