Phase transition, elastic and thermophysical study of Plutonium monochalcogenides under high pressure

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A theoretical study of the high pressure behavior, elastic and various thermo-physical properties of plutonium monochalcogenides using three-body interaction potential (TBIP) model is carried out. The TBIP includes long range Coulombic, three body interaction forces and short range overlap repulsive forces operative up-to next nearest neighbor ions. A static simulation technique including three body interaction effects has been used to investigate phase transition pressures, volume collapses, elastic behavior, stability criteria and various thermo physical properties at high-pressures. The results found are well suited with available experimental data.

1. Introduction

The structural transformation which occurs under pressure in lanthanide and actinide compounds has attracted a wide attention due to large changes of the bulk and electronic properties. Pressure plays a significant role in studying the nature of *f*-electron based lanthanide (4*f*) and actinide (5*f*) systems. As the nature of *f*-electron states depends on the *f*-orbital overlaps, these can be tuned in a controlled manner by changing the interatomic distances by applying external pressure [1, 2]. In that work they had used an interionic potential theory with modified ionic charge, at high pressure but ignored the three –body interaction effect. In present work we have applied the interaction model which includes three –body interaction effect. This influences the physical properties of the *f*-electron based systems and studies on pressure effects in these systems appear to be quite exciting. Since the electronic structure determines the ground state atomic arrangements, studies on crystal structures provide valuable information on the underlying electronic structure [3]. A study of the pressure induced structural changes and relative stability of structures has become very important as it provides an insight in probing their electronic structure, in understanding the transition mechanisms and in predicting phase transition pressure [4]. However, the handling of the actinide systems puts severe restrictions in investigating their properties due to radioactivity. Plutonium (Pu) is considered to be the last member where 5*f* electrons are involved in the metallic bonding at normal temperature and pressure [4, 5]. Thus, there is a special interest in compounds of Pu to determine what effect of pressure may have on the 5*f* electrons in compounds of Pu. It is well known that the effect of pressure changes the

interatomic distance and at particular pressure the coordination number of the compound also changes.

The Plutonium monochalcogenides (PuX: X=Se, Te) display a variety of anomalous physical properties [6]. The PuX crystallize in NaCl structure are of particular interest among the actinides because in contrast to the uranium and neptunium monochalcogenides, magnetic order is absent in the Pu compounds and their lattice constant is anomalous [7]. From the resistivity and the Hall effect data below 300K, PuX were described as small gap semiconductors [8]. In PuX, when the 5*f* electrons treated as itinerant they were found to be relativistic semiconductors with small gaps (0.2-0.4 eV) originating from the spin-orbit spitting of the 5*f* states in two sub-bands [4]. Wachter *et al*. [8] suggested that the PuX are intermediate valent and they are viewed as the high pressure collapsed phase of the divalent samarium chalcogenides. Sanyal et al [1] investigated the structural and elastic properties of PuX using inter ionic potential theory with modified ionic charge at high pressure. Hasegawa and Yamagami [9] made self-consistent linearized augmented plane-wave (LAPW) calculations for PuTe and found it to be semi-metallic. The anomalous properties of the PuX are investigated on the basis of electronic structure calculations. A high-pressure X-ray experiment shows that a structural NaCl-CsCl phase transition occurs in PuTe at 15 GPa with a volume collapse of 9% [10].

Lui et al [11] studied the B1 to B2 pressure induced phase transition in case of PuTe and found phase transition pressure at 14.8 GPa with out spin orbit coupling (SOC) and at 31.7 GPa with SOC. An investigation into the structural phase transition, electronic and optical properties of PuSe under high pressure was conducted by using full potential linearized augmented plane wave local

orbitals (FP-LAPW+lo) in the presence and in absence of SOC [12].

In case of actinide monochalcogenide compounds modeling is a difficult task and this must be guided by experimental evidence to get the suitable model. For experimentalists guidance from theoretical prediction is useful. The only way is to predict at least the extent of pressure one should generate to observe a structural phase transition and their allied properties. Hence, we have employed our TBIP [13, 14] approach to study high pressure behavior in case of actinide monochalcogenides. This approach includes the long range Columbic, three body interaction (TBI) and short range overlap repulsive interaction operative up to second neighbor ions [15].

2. Potential model and method of calculation

It is well known fact that the application of pressure on crystals results in reduction in its volume which leads to an increased charge transfer (or three body interaction effects) [13-15] due to the deformation of overlapping electron shells of the adjacent ions. These effects have been incorporated in the Gibbs free energy (G = U + PV - TS) as a function of pressure (P) [14, 15]. Here U is the internal energy, which at T = $0K$ is equivalent to the lattice energy and S in the vibrational entropy. The Gibbs free energies for rock salt (B1 real) and CsCl (B2; hypothetical) structures at T = 0K and t mbient pressure are given by

$$G_{B1}(r) = U_{B1}(r) + PV_{B1} \qquad (1)$$

$$G_{B2}(r') = U_{B2}(r') + PV_{B2} \qquad (2)$$

In Eqns. (1) and (2) V_{B1} (= $2.00r^3$) and V_{B2} (=$1.54r^3$) are the unit cell volumes for B_1 and B_2 phases respectively. The first terms in the equations (1) and (2) represents lattice energies for B1 and B2 structures and they are expressed as [14, 15]

$$U_{B1}(r) = [-(\alpha_m z^2 e^2)/r] - [(12\alpha_m z e^2 f(r))/r] + 6b\exp[(r_i + r_j - r)/\rho]$$
$$+ 6b\exp[(2r_i - 1.41r)/\rho] + 6 \, b\exp[2r_j - 1.41r)/\rho] \qquad (3)$$

$$U_{B2}(r) = [-(\alpha'_m z^2 e^2)/r'] - [(16\alpha'_m z e^2 f(r'))/r'] + 8b\exp[(r_i + r_j - r')/\rho]$$
$$+ 3b\exp[(2r_i - 1.154r')/\rho] + 3b\exp[2r_j - 1.154r')/\rho] \qquad (4)$$

These lattice energies consists of long-range coulomb energy [first terms in Eqns. (3) and (4), three-body interactions corresponding to the nearest neighbor separation r (r′) for B1 (B2) structures [second terms in equations (3) and (4) and energy due to the overlap repulsion represented by Hafemeister and Flygare (HF) type potential [14] and extended up to the second neighbour ions (rest of the terms). Here, r_i and r_j are the

ionic radii, ρ, b and $f(r)$ are the range, hardness and three body interaction parameters. In Eqn. (3) and (4) three- body potential parameter depends on inter ionic separation and expressed as $f(r) = f_0 e^{-r/\rho}$ with f_0 being a constant. Three model parameters are used in Eqns (3) and (4) viz. $[\rho, b, f(r)]$ the value of which have been determined from the knowledge of the cohesive energy U(r)) and its first order derivative following the equilibrium condition given below. The range parameter (ρ) defines the distance from which the short range repulsive force start to act. The three body interaction parameter $f(r)$ decreases exponentially with the increase of inter ionic separation as defined $f(r) = f_0 e^{-r/\rho}$ [13]. Similarly, hardness parameter (*b*) which is the constant of short range repulsive term in the Eqns (3) and (4) and it denotes strength of force.

$$[\frac{dU}{dr}] = 0 \quad \text{and}$$

$$B_1 + B_2 = -1.165 \, z \, (z + 12f(r)) \qquad (5)$$

Here B_1 and B_2 are the first and second–order derivatives of the short range potentials. In order to probe the elastic behavior of the proposed compounds we have calculated the second order elastic constants (SOEC's), their pressure derivatives and the third order elastic constants (TOEC's). These elastic constants will provide the knowledge of interionic forces in the crystal [16]. These SOEC's are functions of the first and second–order derivatives of the short range potentials their calculation will provide the effect of short range forces in these materials. The basic theory for deducing the expressions of the second, third and higher order elastic constants is described in [16, 17]. We have obtained SOEC's, their pressure derivatives and third order elastic constants with the help of relations given in [18]. Moreover, the third order elastic constants *(*TOECs) furnish accurate information about the repulsive interactions as their contributions are dominant in the higher derivatives of the potential energy. The TOECs furnish important regarding the thermal expansion and the temperature and pressure dependence of SOEC.

Exploiting the TBIP model we have calculated various thermo physical properties of PuX compounds. We have calculated the compressibility (β), molecular force constant (f), infra red absorption frequency (ν_0), Debye temperature (Θ_D), Gruneisen parameter (γ) and anharmonicity (*A*) of these compounds. These thermo physical properties provide us the interesting information about substances viz, the Debye temperatuture (Θ_D) explores the structural stability, dislocations in structure and the strength of bonds between the elements. The

expressions of these thermo- physical are taken from [19, 20]

In the same sequence compressibility (β) is given by well known relation

$$\beta = \frac{3Kr_0}{f} \qquad (6)$$

where molecular force constant (*f*) is

$$f = \frac{1}{2}\left[\Phi^{SR}_{kk\cdot}(r) + \frac{2}{r}\Phi^{SR}_{kk\cdot}(r\cdot)\right] \qquad (7)$$

Here, $\Phi^{SR}_{kk\cdot}(r)$ are the short range nearest neighbor part which is given by the last three terms in the Eqns.(3) and (4). This force f leads to the infrared absorption frequency which is deduced by the knowledge of the reduced mass (μ).

$$\nu_0 = \frac{1}{2\pi}\left[\frac{f}{\mu}\right]^{1/2} \qquad (8)$$

This frequency is utilized to calculate the Debye temperature as follows

$$\Theta_D = \frac{h\nu_0}{k}$$

where *h* and *k* are the Plank and Boltzman constants respectively.

The important Gruneisen parameter (γ) [20] is given by

$$\gamma = -\frac{r_0}{6}\left[\frac{\Phi'''_{kk\cdot}(r)}{\Phi''_{kk\cdot}(r)}\right] \qquad (9)$$

Here, $\Phi'''_{kk\cdot}(r)$ and $\Phi''_{kk\cdot}(r)$ are the third and second derivatives of cohesive energy. The PuX compounds are cubic which is isotropic in nature but also has elastic anisotropy due to the presence fourth rank tensor elastic property. The elastic anisotropic parameter of a cubic crystal is defined in [20] as

$$A = \left[\frac{2C_{44} + C_{12}}{C_{11}}\right] - 1 \qquad (10)$$

3. Result and discussion

We know that an isolated and stable phase is always associated minimum of energy. So the promising technique of minimization of $GB1(r)$ and $GB2(r\cdot)$ at different pressures is utilized in order to obtain the interionic separations r and $r\cdot$ corresponding to $B1$ and $B2$ phases. Input and model parameters used in Eqns. (3) and (4) are well tabulated in Table 1. The change in Gibb's

free energies $\Delta G = (GB2(r\cdot) - GB1(r))$ are plotted against pressure (*P*) and are shown in Fig. 1 for PuSe and PuTe. The difference in Gibbs free energies ΔG in real (B1) and hypothetical (B2) phases is an important factor in predicting the phase transition pressure. The phase transition pressure (P_t) is the pressure at which ΔG approaches zero [13, 14]. After phase transition B1 phase becomes hypothetical and B2 phase becomes real. It is shown in Fig. 1 that the phase transition pressures for PuSe and PuTe are 34.9 GPa and 14.8GPa respectively which are close to the experimental phase transition pressure 35 GPa [3] and 15-19 GPa [10] as given in Table 3. Concisely we point that from TBIP model the estimated value of P_t are in good agreement with experimental and other theoretical works which are listed in Table 3.

Table 1. Input data.

Comp.	r_i (Å)	r_j (Å)	r_0 (Å)
PuSe	1.00 [a]	1.3 [a]	2.8996 [a]
PuTe	1.00 [a]	1.3 [a]	3.0872 [b]

[a]Ref. [3], [b]Ref. [10]

Table 2. Model parameters for Plutonium monochalcogenides.

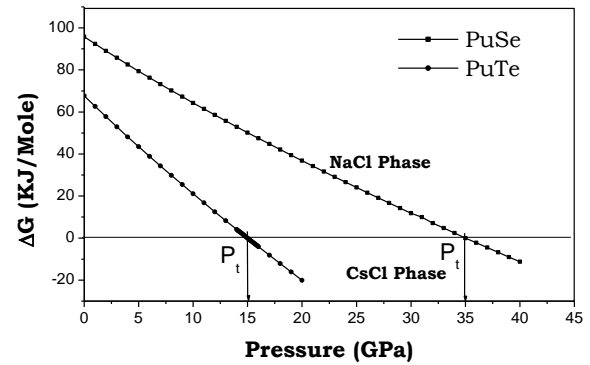| Comp.	b(10^{-19}J)	ρ(Å)	f(r)
PuSe	2.806717	0.339414	-0.0094017
PuTe	5.7961	0.28887	-0.0075193

Fig. 1. Variation of Gibbs free energy with pressure.

Furthermore, usually experimentalists the compressions are investigated through associated volume changes and a sudden collapse in volume at phase transition pressures. This sudden change in volume occurs from the change in atomic arrangement during phase transition leading to new structure. Also the discontinuity in volume at phase transition pressure confirms the occurrence of first order phase transition. The estimated relative volume changes [$\Delta V(P)/V(0)$] are plotted with various high pressures for PuSe and PuTe as shown in Fig.

2. The magnitude of relative volume changes at the transition pressure for PuSe and PuTe are 7.8 %, and 11.8 % respectively which are very close to the experimental works [3, 10] than earlier works [1].

Table 3. Phase transition and volume collapse.

Comp.	Phase Transition Pressure (GPa)				Volume Collapse (%)		
	Present	Others		Exp.	Present	Others	Exp.
PuSe	34.9	37.1[c]	36.3[d]	35 [a]	7.8	5.5[c]	11 [a]
PuTe	14.8	17.9[c]	31.7[e]	15-19 [b]	11.8	6.4[c]	9 [b]

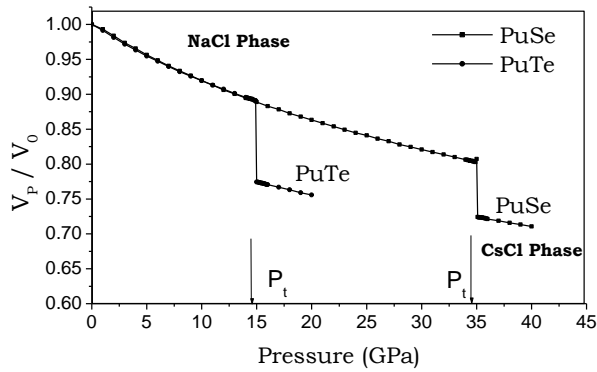[a]Ref.[3] ,[b]Ref. [10], [c]Ref.[1] [d]Ref.[12] [e]Ref.[11]

Fig. 2. Variation of relative volume with pressure.

The information of Elastic constants and their pressure derivatives are important as they help us to understand the interatomic forces in solids. We have applied the lattice theoretical study of second order elastic constants (SOECs) by the method of homogeneous finite deformation. The expressions of SOECs are taken from [20]. The SOECs and their combination $C_L=(C_{11}+C_{12}+2C_{44})/2$, $C_s = (C_{11}-C_{12})/2$ are calculated usig [17, 18] and are listed in the Table 4 and 5. The calculated values of the bulk modulus are also listed in Table 6 which is well suited with the experimental and other work [1, 3, 10]. The variations in the results of elastic constant are due to the inclusion of three-body interaction effect. The pressure derivative of the bulk modulii ($\frac{dB_T}{dP}$), shear-modulii ($\frac{dS}{dP}$) and the trigonal shear elastic modulus ($\frac{dC_{44}}{dP}$) at zero pressure and are listed in Table 5. The cohesive energies for both the phases viz. B1 and B2 are listed in Table 6. The variations of C_{11}, C_{12}, C_{44} and B_T with pressure are shown in Fig. 3 (a), 3 (b) and Fig. 4. Our results are well suited with the first order transition for these PuX- cubic compounds and are similar to the earlier reported elastic stiffness results for ScAs [20], PbTe and SnTe [21] having the NaCl- structure with B1 to B2 structural phase transition Vukcevich [22] stated the

stable phase of a crystal is one in which the tetragonal elastic constant C_{44} is non-zero (for mechanical stability) and which has the lowest potential energy among the mechanically stable lattices. The Born criterion for a lattice to be mechanically stable which states that the elastic energy density must be a positive definite function of strain. This requires that the principal minors (the eigen values) of the elastic constant matrix should all be positive. Thus using both the above defined stability criterion for NaCl structure in terms of the elastic constants which are followed by Singh et. al. [14, 15] are

$$B_T = \frac{1}{3}(C_{11} + 2C_{12}) \succ 0 \,, C_S = \frac{1}{2}(C_{11} - C_{12}) \,, C_{44} \succ 0$$
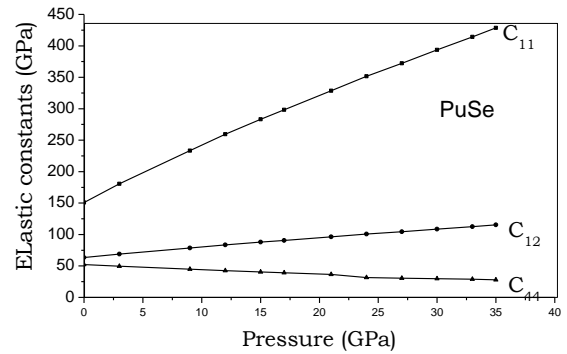

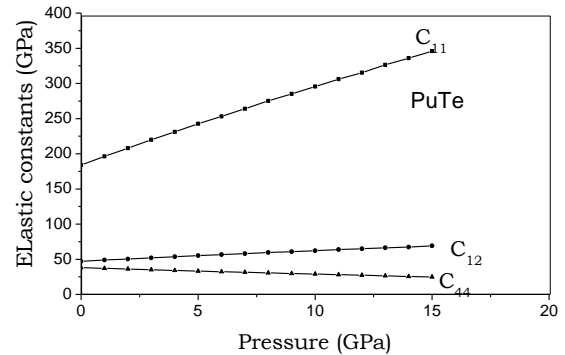*Fig. 3a. Variation of C_{11}, C_{12} and C_{44} with pressure (GPa) for PuSe.*

Fig. 3b. Variation of C_{11}, C_{12} and C_{44} with pressure (GPa) for PuTe.
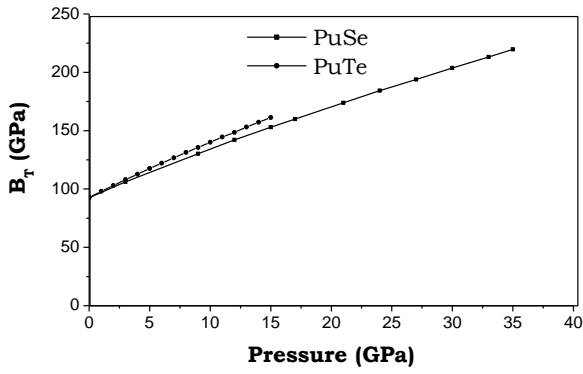
Fig. 4. Variation of B_T with Pressure (GPa).

Here the C_{44} and Cs are the tetragonal and shear modulus of a cubic crystal. It is well inferred from the Table 3 and 4 that the above defined stability criterion are well suited for these PuX compounds using the TBIP. It is clear from Table 4 that the value of C_{44} for PuSe and PuTe are positive and hence satisfy the stability condition by Vukcevich [22]. Demarest et al. [23] proposed a slight modification of the Born stability criterion that a phase transition take place when the ratio $\frac{C_{44}}{B_T}$ reaches a critical value in the neighborhood of 0.14 and 0.2. Table 4 shows that we have obtained the same trends from TBIP and hence also well satisfied the above stability criterion. We have also shown the trends of $\frac{C_{44}}{B_T}$ with pressure and shown in Fig. 5. The trends of $\frac{C_{44}}{B_T}$ for these PuX compounds decrease with pressure but could not reach zero up to phase transition pressure as defined above. This shows that our calculated elastic constants with this TBIP are well suited with the above stability criterion [23]. It is true that the comparison of the experimental and theoretical results is not possible since these compounds are recently discovered.

Table 4. The calculated values of elastic constants SOEC's (10^{12} dyne/cm^2).

Comp.	C_{11}		C_{12}		C_{44}		C_{44}/B_T
	Present	Others	Present	Others	Present	Others	Present
PuSe	1.50	2.10	0.63	0.34	0.522	0.34	0.12
PuTe	1.83	1.09	0.47	0.16	0.38	0.16	0.15

[a]Ref.[1]

Table 5. Variation of second order elastic constants with pressure and combination of SOEC`s.

Comp.	$\dfrac{dB_T}{dP}$	$\dfrac{dS}{dP}$	$\dfrac{dC_{44}}{dP}$	Cs = (C$_{11}$-C$_{12}$)/2 (10^{12} dyne/cm^2)	C$_L$=(C$_{11}$+C$_{12}$+2C$_{44}$)/2 (10^{12} dyne/cm^2)
PuSe	4.916	3.600	-0.056	0.492	1.59
PuTe	5.570	5.110	-0.359	0.683	1.53

Table 6. Calculated bulk modulus and cohesive energy.

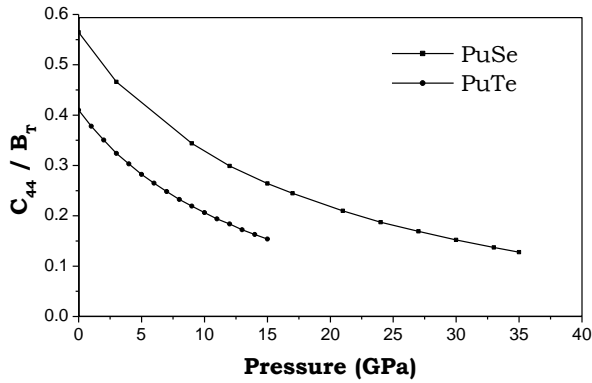| Comp.	B_T (GPa)		$\mu(10^{-24}$ g)	Cohesive energy	
	Present	Exp./others		U$_1$ (B$_1$) kJ/mole	U$_2$(B$_2$) kJ/mole
PuSe	92.5	98 [a]/92[c]	98.52880	-3010.36 (-2178.91)[a]	-2914.59 (-2099.38)[a]
PuTe	92.82	34 [b]/47[c]	138.10069	-2894.49 (-1261.91)[a]	-2826.79 (-1261.9)[a]

[a]Ref.[3] ,[b]Ref. [10], [c]Ref.[1]

Fig. 5. Variation of C_{44}/B_T with Pressure (GPa).

Moreover the calculated values TOEC's from TBIP at zero pressure are given in the Table 7 for PuSe and PuTe. It is clear from Table 7 that the $C_{111}, C_{112}, C_{166}$ are negative while that of $C_{123}, C_{144}, C_{456}$ are positive. The present studies on TOEC's reveal that their behavior is just opposite to the behavior of SOEC. It is also evident from the experimental values of TOEC's for alkali halide viz. NaCl, KCl, etc that the Cauchy discrepancies among the TOEC's are not very large and are of about the same order as those among the SOEC, viz. $(C_{11} - C_{12})$. This result, according to our present TBIP is shown better resemblance which is most inspiring for experimentalists. However the experimental studies on the TOEC's of the system of solids under consideration are relatively difficult and only measurement available up to present date are the pressure derivatives of the SOEC.

Table 7. Calculated third order elastic constants.

Comp.	C_{111}	C_{112}	C_{123}	C_{144}	C_{166}	C_{456}
PuSe	25.3622	-2.88	1.06650	0.87047	-2.0849	0.84546
PuTe	-34.2494	-2.2179	0.83792	0.6823	-1.49516	0.6658

The various important thermo physical properties viz compressibility (β), Debye temperature (Θ_D), Gruneisen parameter (γ) and anharmonicity (A) are well tabulated in Table 8 exploiting the most appropriate TBIP model. Compressibility of crystal relates the relative volume change of crystal as a response to pressure change [16, 17]. From Table 8 it is clear that the values of β are near about unity in case of PuSe and PuTe. The Debye temperatures are calculated from well known Blackman formula and their values for PuSe and PuTe are 204.8K and 201.32 respectively. The Debye temperature is important property as it relates to many physical properties viz. the specific heat, melting temperature and also it estimates the phonon contribution to specific heat [20]. It is seen that at low temperature the vibration excitations arise only from acoustic vibrations. Hence at low

temperature the value of Θ_D calculated from elastic constants is the same as that determined from specific heat measurements [20]. Direct evidence of experimental values for the Debye temperature of solids under study is not known yet but our results are closed to same class of compound viz. LaBi [24]. We have calculated the Gruneisen parameter (γ) which relates how the vibration frequency (phonons) within a crystal is altered with changing volume. Also, our values of Gruneisen parameter (γ) seem to be more realistic as they are close in magnitude to the measured values of alkali halides and other monochalcogenides having NaCl type structure [13]. The elastic anisotropy factor (A) is well used in the interpretation of the seismological and shear wave velocities. It is well inferred from Table 8 that the PuSe and PuTe are anisotropic as their values are single valued and small positive.

Table 8. Calculated thermo-physical properties.

Comp.	f (10^5 dyne cm^{-1})	v_0 (10^{12} Hz)	β (10^7 dyne cm^{-1})	v_0 (10^{12} Hz)	Θ_D (K)	γ	A
PuSe	7.13957	4.282	1.11	4.282	204.81 (205)[a] (178)[b]	1.48	1.083
PuTe	7.734106	3.764	1.09	3.764	201.32	1.81	0.663

[a]Ref. [20], [b]Ref. [24]

4. Conclusions

In the present study, we have developed a TBIP approach to investigate the structural, elastic and stability

conditions of plutonium compounds. The results are summarized as follows:

1. Our results with present approach including TBI effect are showing good matching with experimental results and other theoretical results.
2. Our relative volume changes for these compounds are well suited with the experimental results.
3. We have predicted the correct cohesive energies including TBI.
4. The stability criterion under pressure which is important tool for geologist to work with these compounds is studied for the first time successfully.
5. We have calculated important physical properties like compressibility (β) Debye temperature (Θ), Grunneisen parameter (γ) and Anharmonicity (A).

It is thus obvious from the overall study that the present TBIP model is adequately suitable for describing the phase transition and the modified stability criterion for these compounds. Thus TBIP model promises successful description of high pressure studies in case of recently discovered actinide compounds series.

Acknowledgment

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