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Temperature variation of anharmonic properties of Thorium Sulphide

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Abstract
For Thorium sulphide; the elastic energy density is expanded as a power series of strains using Taylor series expansion starting from nearest neighbour distance and hardness parameter using Coulomb and Born Mayer potentials for obtaining higher order elastic constants. The higher order elastic constants for a crystal are useful for obtaining the anharmonic properties of crystal within the limit of the continuum approximation in a quantitative manner. Thorium sulphide crystal possesses face centered crystal structure. For obtaining second, third and fourth order elastic constants of Thorium sulphide crystal at elevated temperature are computed. These elastic constants are used to evaluate their pressure derivatives. The results are discussed.

Keywords: *Elastic constants, Anharmonicities, partial contraction.*

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I. INTRODUCTION

Anharmonic properties of Thorium compounds using long range Coulomb and short range Born Mayer potentials (1-4). The elastic energy density for a deformed crystal is expanded as a power series of strains, the coefficient of quadratic, cubic and quartic terms are known as the second, third and fourth order elastic constants respectively. When the values of these elastic constants for a substance are known; many of the anharmonic properties of the solid can be treated with in the limit of the continuum approximation in a quantitative manner.

Anharmonicities such as specific heat at higher temperature, thermal expansion, temperature variation of ultrasonic velocity and attenuation, first order pressure derivatives of second order elastic constants, Grüneisen numbers and temperature derivatives of second order elastic constants are directly related to second and third order elastic constants (5-8). While discussing higher order anharmonicities such as the second order pressure derivatives of second order elastic constants, the first order elastic constants, partial contractions and deformation of solids under large forces, the fourth order elastic constants are to be considered extensively. Some few efforts have been made for obtaining fourth order elastic constants of materials having different crystal structures.

Some work has been done by various investigators while studying the anharmonic properties of solids of several types (9-10). The present theory deals with the formulation for obtaining SOEC, TOEC and FOECs at any temperature, the first order derivatives of second order elastic constant and third order elastic constant, second order pressure derivatives of second order elastic constant and partial contractions using long and short range potentials starting from the nearest neighbour distance and repulsive parameter (11).

Formulation

The elastic energy density for a crystal of a cubic symmetry can be expanded up to quartic terms as;

$U_0 = U_2 + U_3 + U_4$

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

Where C_{ijkl}, C_{ijklmn} and $C_{ijklmnpq}$are the second order elastic constants , third order elastic constants and fourth order elastic constants in tensorial form , X_{ij} are the Lagrangian strain components, C_{ij} , C_{ijk} andC_{ijkl} are the SOECs , TOECs and FOECs in Bruggr,s definition and Voigt notations.

$C_{ijkl} = C_{IJ} = (\partial^2 U/\partial X_{ij}\partial X_{kl})_{x = 0}$

$C_{ijklmn} = C_{IJK} = (\partial^3 U / \partial X_{ij}\partial X_{kl}\partial X_{mn})_{x=0}$

And $C_{ijklmn} = C_{IJKL} = (\partial^4 U/\partial X_{ij}\partial X_{kl}\partial X_{mn}\partial X_{pq})_{x=0}$ (2)

The free energy density of a crystal at a finite temperature T is

$U_{total} = U_0 + U^{vib}$ (3)

Where U_o is the internal energy per unit volume of the crystal when all ions at rest on their lattice points, U^{vib} is the vibrational free energy.

$C_{IJ} = C_{IJK}{}^{0} + C_{IJK}{}^{vib}$

And,$C_{IJKL}=C_{IJKL}^{0}+C_{IJKL}^{vib}$ (4)

The first part is the strain derivatives of the internal energy U_0 is known as static elastic constants and second part is the strain derivative of the vibrational free energy U^{vib} is called vibrational elastic constant.

Evaluation

For the calculation of many anharmonic properties of the substances possessing FCC crystal structures is given in the initial section. The TOECs for ThS is evaluated at 300 K temperature. Selecting a few data obtained in this study, the values of TOECs at room temperature are given in table. The order pressure derivatives of SOEC and TOEC and second order pressure derivatives of SOEC have been evaluated and results are shown in Table. The evaluation is mainly based on the FCC crystal structure of material does not change when temperature varies. The values of the nearest neighbor distance (r_0) and hardness parameter q are given in Table.

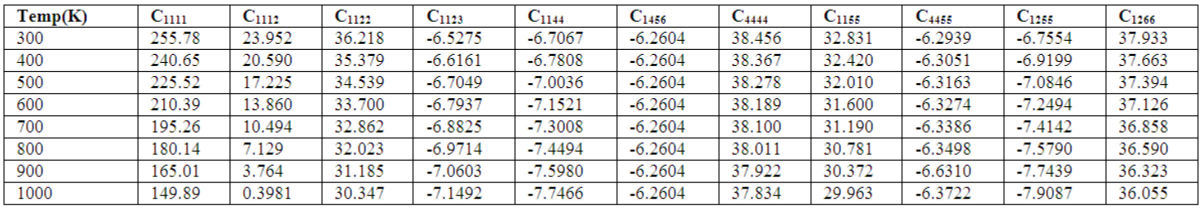
II. RESULT AND DISCUSSION

The second, third and fourth order elastic constants (SOEC, TOEC and FOEC) have been calculated using basic parameters i.e., nearest neighbour distance (r_0) and hardness parameter (q) for thorium sulphide. The theory of many nonlinear properties of the compounds possessing FCC crystal structures is pre existing part. The TOECs for ThS is computed from temperature varying from 300 K to near about melting point temperature. FCC crystal structure of ThS is shown with the temperature variation. The data required for the study is given in tables 1 to 4. The SOECs and TOECs of ThS are computed with the variation of temperature in table 1 using basic parameter. Future we calculated FOECs of ThS in 10e12 dyne/cm2 varying the temperature. In table 3 FOPDs of SOECs and TOECs are evaluated. Similarly the SOPDs of SOECs and partial contraction have been obtained with the variation of temperature in table 4. Due to lack of experimental data related to present study obtained data cannot be compared theoretically. Finally we can say all elastic constants and their pressure derivatives have a dependence upon the variation of temperature. These graphs show temperature variation for different elastic constants, their pressure derivatives and partial contraction of ThS substance. By these graphs it can be said obviously that SOECs is directly proportional to temperature. The graph between TOECs and temperature is a line parallel to temperature line it means that with the variation of temperature TOECs has a little bit change. By the graphs between FOECs and temperature it is clear as the temperature increases FOECs decreases. A FOPD of SOECs increase with the temperature varies slowly. The graph between partial contraction and temperature shows that the relation between these two is of inversely proportionality.

Table 1-The SOECs and TOECs in 10^{11} dyne/cm^2 of ThS.

Temp(K)	C_{11}	C_{12}	C_{44}	C_{111}	C_{112}	C_{123}	C_{144}	C_{166}	C_{456}
300	20.746	18.425	18.635	-245.35	10.8700	28.689	27.516	21.180	26.794
400	21.484	18.375	18.653	-244.00	08.3260	29.318	27.756	21.302	26.794
500	22.237	18.325	18.671	-242.69	05.6533	29.948	27.996	21.421	26.794
600	22.998	18.275	18.690	-241.39	02.9144	30.578	28.236	21.538	26.794
700	23.763	18.226	18.709	-240.11	0.1370	31.208	28.477	21.655	26.794
800	24.532	18.176	18.728	-238.83	-2.6646	31.839	28.717	21.772	26.794
900	25.302	18.126	18.747	-237.56	-5.4825	32.409	28.957	21.888	26.794
1000	26.074	18.077	18.766	-236.29	-8.3119	33.100	29.198	22.005	26.794

Table 2- The FOECs of ThS in 10^{12} dyne/cm^2



Temp(K)	C_{1111}	C_{1112}	C_{1122}	C_{1123}	C_{1144}	C_{1456}	C_{4444}	C_{1155}	C_{4455}	C_{1255}	C_{1266}
300	255.78	23.952	36.218	-6.5275	-6.7067	-6.2604	38.456	32.831	-6.2939	-6.7554	37.933
400	240.65	20.590	35.379	-6.6161	-6.7808	-6.2604	38.367	32.420	-6.3051	-6.9199	37.663
500	225.52	17.225	34.539	-6.7049	-7.0036	-6.2604	38.278	32.010	-6.3163	-7.0846	37.394
600	210.39	13.860	33.700	-6.7937	-7.1521	-6.2604	38.189	31.600	-6.3274	-7.2494	37.126
700	195.26	10.494	32.862	-6.8825	-7.3008	-6.2604	38.100	31.190	-6.3386	-7.4142	36.858
800	180.14	7.129	32.023	-6.9714	-7.4494	-6.2604	38.011	30.781	-6.3498	-7.5790	36.590
900	165.01	3.764	31.185	-7.0603	-7.5980	-6.2604	37.922	30.372	-6.6310	-7.7439	36.323
1000	149.89	0.3981	30.347	-7.1492	-7.7466	-6.2604	37.834	29.963	-6.3722	-7.9087	36.055

Table 3- The FOPDs of SOECs and TOECs of ThS.

Temp(K)	dC_{11}/dP	dC_{12}/dP	dC_{44}/dP	dC_{111}/dP	dC_{112}/dP	dC_{123}/dP	dC_{144}/dP	dC_{166}/dP	dC_{456}/dP
300	-2.7108	-1.8352	-2.5367	-36.9473	-10.8796	2.9056	1.0769	-3.4576	2.8651
400	-2.6781	-1.6359	-2.5285	-32.8263	-9.9037	2.8979	1.1238	-3.2879	2.8447
500	-2.6475	-1.6341	-2.5199	-28.7832	-8.9398	2.8900	1.1691	-3.1208	2.8242
600	-2.6185	-1.5320	-2.5114	-24.8245	-7.9927	2.8820	1.2132	-2.9568	2.8039
700	-2.5906	-1.4308	-2.5028	-20.9507	-7.0641	2.8741	1.2562	-2.7961	2.7840
800	-2.5636	-1.3310	-2.4944	-17.1607	-6.1543	2.8662	1.2981	-2.6388	2.7644
900	-2.5373	-1.2327	-2.4861	-13.4525	-5.2634	2.8584	1.3391	-2.4847	2.7412
1000	-2.5118	-1.1363	-2.4780	-9.8241	-4.3911	2.8509	1.3791	-2.3340	2.7264

Table 4: The SOPDs of SOECs in 10^{-12}dyne/cm^{2}and Partial Contraction in 10^{13} dyne/cm^2

Temp(K)	**d^2C_{11}/dP^2**	**d^2C_{12}/dP^2**	**d^2C_{44}/dP^2**	**Y_{11}**	**Y_{12}**	**Y_{44}**
300	11.021	1.4331	3.5955	41.097	8.7703	10.780
400	10.149	1.2237	3.3306	38.054	7.8858	10.563
500	9.332	1.0294	3.0665	35.009	7.3070	10.346
600	8.558	0.8853	2.8089	31.965	6.1154	10.130
700	7.825	0.7023	2.5603	28.920	5.2301	9.914
800	7.128	0.5700	2.3213	25.876	4.3448	9.787
900	6.464	0.4575	2.0922	22.830	3.4595	9.482
1000	5.832	0.3635	1.8729	19.788	2.5744	9.266

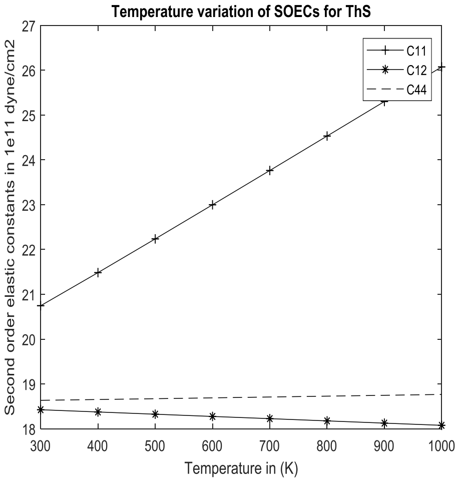
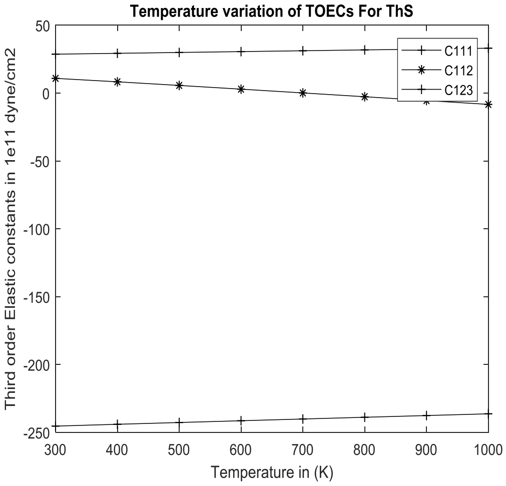


Fig 1



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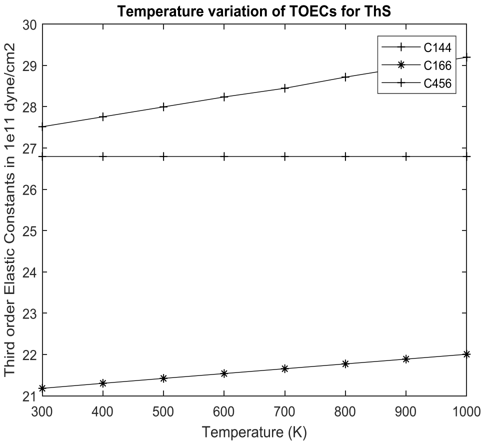

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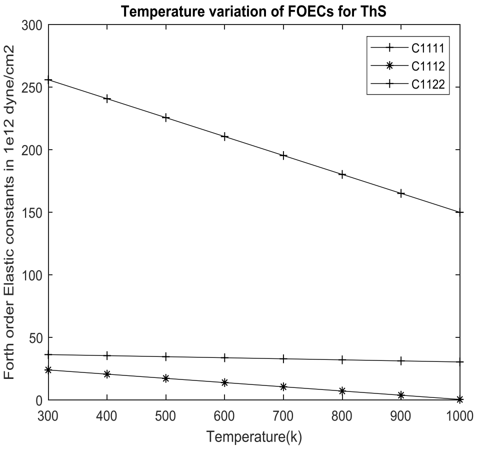

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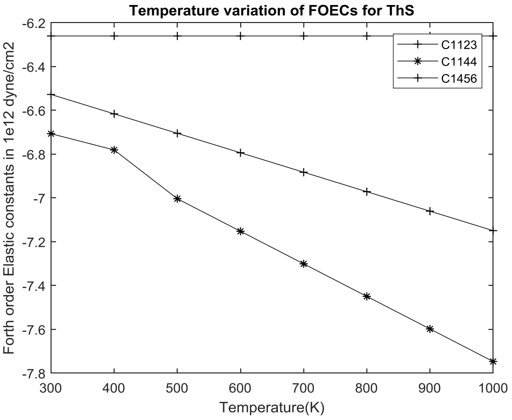

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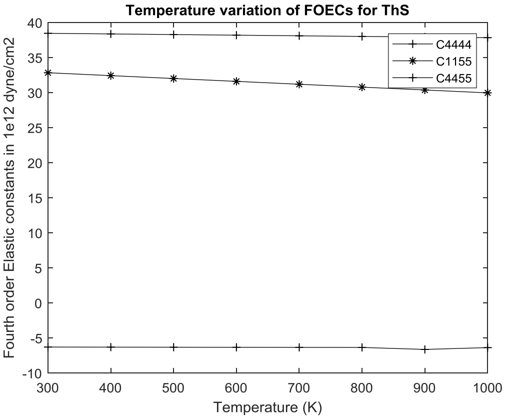

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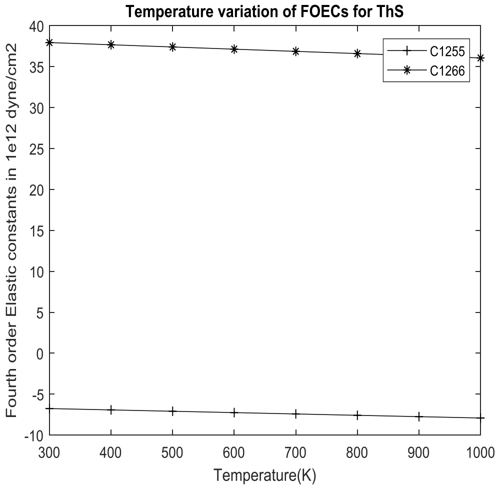

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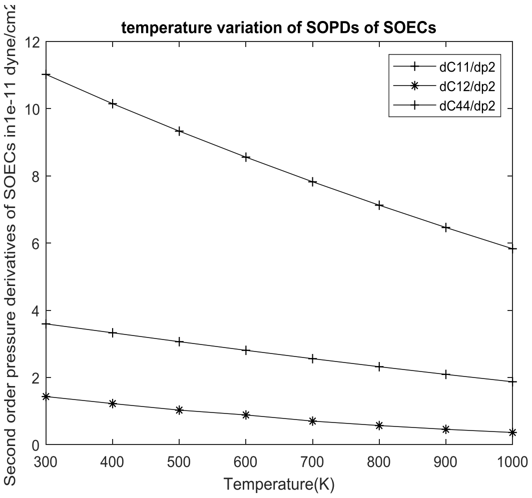

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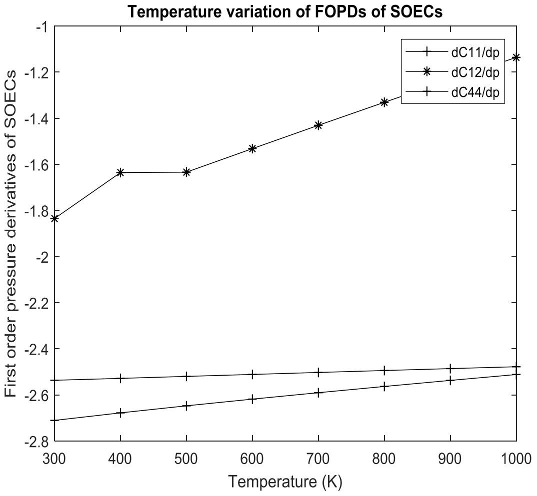

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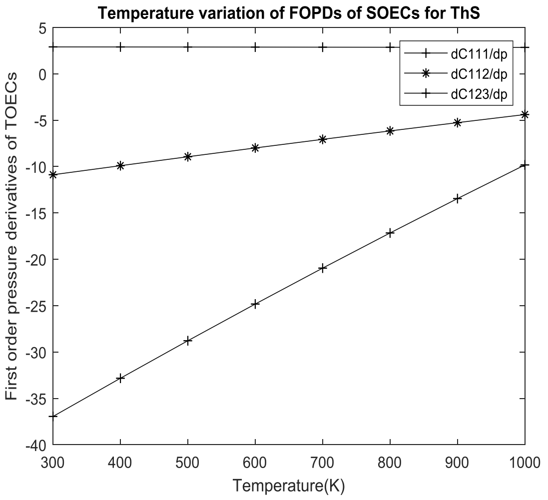

fig10

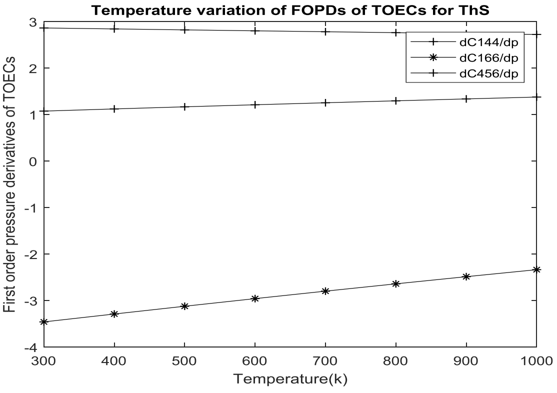

Fig 11

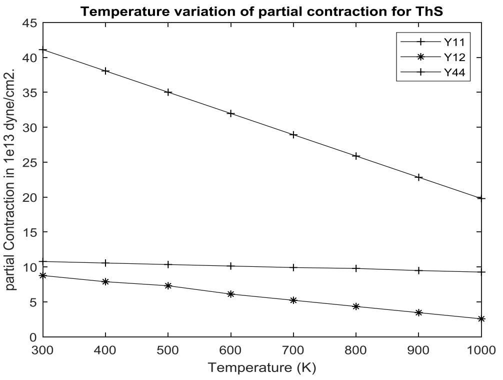

fig 12

III. CONCLUSION

The elastic constants of Thorium compound are varying as temperature varied. Some nonlinear properties are also computed using elastic constants data.

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