International Journal of Advance Research in Science and Engineering
Vol. No.9, Issue No. 09, September 2020
www.ijarse.com
IJARSE
ISSN 2319 - 8354

Structural and Mechanical Properties of Thorium Oxide

Nilesh Dhurve[1*], Neetu Paliwal[2]

[1]*Department of Physics, Govt. College, Bhimpur, Betul- 460330, India*

[2]*Department of Physics, Rabindranath Tagore University, Bhopal 464993, India*

Abstract

We have investigated the cohesive energies, equilibrium lattice constants, pressure-volume relationship, phase transition pressure and elastic constant for thorium oxide using an interionic potential theory with modified ionic charge, which includes Coulomb screening effect due to d-electrons. This compound undergoes structural phase transition from NaCl (B_1) to CsCl (B_2) structure at high pressure 65 GPa. We have also calculated bulk, Young, and shear moduli, Poisson ratio and anisotropic ratio in NaCl (B_1) structure and compared them with other experimental and theoretical results which show a good agreement.

Keywords: B_1-B_2 Phase transition; Mechanical properties of solid.

1 Introduction

Thorium compounds have attracted much attention due to their chemical and physical properties making them interesting from the fundamental point of view as well as for a variety of applications. The potential of utilizing of these compounds as an alternative or supplement for uranium compounds has been acknowledged for long time. Importantly, various types of reactors have already operated using thorium compounds based fuels. Currently the significance of thorium compounds remains strong and growing concerns over nuclear reactor waste, safety and proliferation. These compounds may be used in solid fuel form or in molten form [1-3]. The high pressure structural behaviour, equation of state and electronic structure calculation of thorium and

compounds has received some importance in the past. Recent studies using synchrotron and powder X-ray diffraction at high pressure indicated that under pressure, a number of binary rare earth compounds with NaCl-type (B_1) structure undergo a phase transition to CsCl-type (B_2) structure. Shein et al. [4] have studied the electronic structure of cubic ThC, ThN, and ThO using the FP – LAPW + lo method within the GGA. For perfectly stoichiometric ThN, they found good agreement with experimental values for the lattice constant, bulk modulus, and specific heat coefficient. They also noted that the bonding behaviour of the ThX (X = C, N, and O) phases is a linear combination of covalent, ionic, and metallic characters. In the present study we have investigated the structural and mechanical properties of thorium oxide at ambient and high pressure using interionic potential theory with modified ionic charge.

2 Method of Calculation

The interionic potential for the thorium oxide in the frame work of rigid ion model is expressed as [5-9]

$$U(r) = \sum \frac{Z_m^2 e^2}{r_{ij}} + \sum_{ij} b\beta_{ij} \exp\left[\frac{\left(r_i + r_j - r_{ij}\right)}{\rho_{ij}}\right] + \sum_{ij} C_{ij} r_{ij}^{-6} + \sum_{ij} D_{ij} r_{ij}^{-8} \qquad (1)$$

Which includes the long-range Coulomb interaction (first term), Hafemesiter and Flygare form of short range repulsive (second term) and van der Waals multipoles interactions (third and last term). $Z_m e$ is the modified ionic charge and parametrically includes the effect of the Coulomb screening due the d-electron for this compound. b and p are short range parameters, which can be determined from the equilibrium condition. Thermodynamically, a phase transition is said to occur when change in the structural details of the phase are caused by variation of the free energy. ThC transform from their initial NaCl (B_1) to CsCl (B_2) type structure under pressure. The stability of a particular structure is decided by the minima of the Gibbs energy, given by

$$G=U+PV-TS \quad (2)$$

Where U is the internal energy at 0K temperature corresponding to the cohesive energy, S is the vibrational entropy at absolute T, pressure P and volume V.

3 Results and Discussion

Under high pressure the thorium oxide compound undergoes a structural phase transformation from initial NaCl- to CsCl-type. The structural phase transition pressure was found to be 65.0 GPa with relative volume change 7.5%, for ThO. Since no experimental results are available at present hence our calculated results will certainly help the experimentalists to analyze their data in future.

Table 1: Input parameters and generated model parameters for ThO.

Solid	Input parameters			Model parameters			
	r_+ (Å)	r_- (Å)	r_0 (Å)	B_0(GPa)	Z_m^2	b(x 10^{-19}J)	ρ(Å)
ThO	0. 91	1.12	2.556[b]	160.2[b]	3.31	1.031	0.227

The elastic properties define materials, when it undergo stress, deform and then recover and return to its original shape after stress ceases. The elastic properties of a material play an important role in providing valuable information about binding characteristics between the adjacent atomic plane, structural stability, specific heat, thermal expansion, Debye temperature and Grüneisen constant.

International Journal of Advance Research in Science and Engineering
Vol. No.9, Issue No. 09, September 2020
www.ijarse.com
IJARSE
ISSN 2319 - 8354

Table 2: Cohesive energies and phase transition properties for ThO.

Solids		Equilibrium inter-ionic distance (Å)		Cohesive energy KJ/mol		Phase Transition pressure (GPa)
		$R1(B_1)$	$R2(B_2)$	$U1(B_1)$	$U2(B_2)$	P_t
ThO	Present	2.600	2.800	-2902	-2802	65.0
	Expt.	2.651[a]	---	---	---	---
	Other	2.556[b]	---	---	---	---

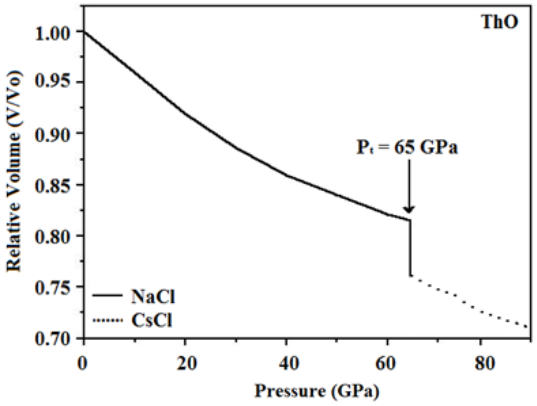

Figure 1: P-V relation for ThO

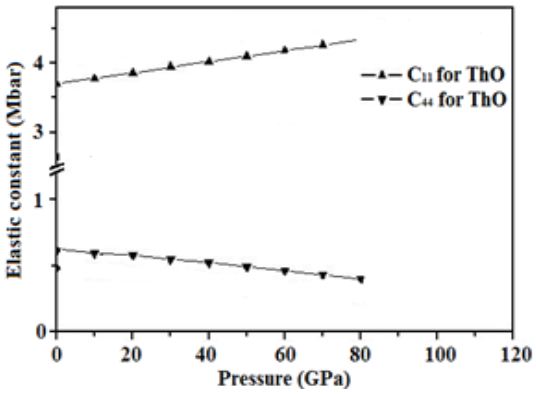

Figure 2: Elastic constants for ThO.

We have calculated the elastic constants of thorium oxide at normal as well as at high pressure. In the case of cubic system, there are only three independent second order elastic constants (SOEC) namely C_{11}, C_{12} and C_{44}. Since we use two-body interaction potential between the species, the calculated values of C_{12} and C_{44} are equal. The calculated values of SOEC are tabulated in Table 1 and compared with other theoretical values [4]. It is clear from Table 2 that the calculated values of equilibrium lattice parameters in NaCl- and CsCl-type structures are in good agreement with available experimental and theoretical results [4]. Equation of states for thorium oxide is presented in Fig. 2. Calculated values of elastic constants are 380, 63, 63 respectively for C_{11}, C_{12} and C_{44}, bulk modulus (B_T) 169, Young modulus (E) 120, shear modulus (G) 101 in (GPa), Poisson ratio (ν) 0.1422 and anisotropic ratio (A) 0.39 for thorium oxide. The stability of ThO can also be defined by the SOEC. We have compared our results to the stability criteria using the following relation:

$$C_{11}\text{-}C_{12} > 0,\ C_{44} > 0,\ B_0 > 0$$

We have found that in NaCl-type structure; these criteria are satisfied, indicating that this phase is elastically stable. We have calculated the pressure dependence of the SOEC, namely C_{11} and C_{44} in Figure 3. It is clear from the Figure 3 that C_{11} varies largely under the effect of the pressure as compared with C_{44}. The elastic constant C_{11} represents the variation of the length with pressure; a longitudinal strain is produced, which brings change in C_{11}.

3 Acknowledgments

The authors are thankful to Higher Education Government of Madhya Pradesh and University Grant Commission (UGC) New Delhi. N. D. is also thankful to V. C. RNTU, Bhopal for support.

4 References

[1] A. J. Freeman, G.H. Lander, Handbook of the Physics and Chemistry of the Actinides, Publisher: Amsterdam, North-Holland, 1985.

[2] M. Aynyas, J. Pataiya, B. S. Arya, A. Singh, and S. P. Sanyal, Structural and mechanical properties of thorium carbide J. of Physics, Con. Series **1665** (2015) 030022-030023.

[3] J. M. Leger. Chalcogenides and pnictides of cerium and uranium under high pressure, Physica **B 190** (1993) 84-91.

[4] I. R. Shein, K. I. Shein, A. L. Ivanovskii, First principle study of B1 like thorium carbide nitride and oxide, J. Nucl. Mat. **353** (2006) 19-26.

[5] M. Aynyas, S.P. Sanyal, P.K. Jha, Structural phase transition and elastic properties of thorium pnictides at high pressure, Phys. Status Solidi **B 229** (2002) 1459-1466.

[6] P. K. Jha, S. P. Sanyal, Structural phase transition and high-pressure behaviour of curium and uranium monobismuthides, J. of physics and Chemistry of Solids **64** (2003) 1237-1240.

[7] P. K. Jha, S. P. Sanyal, Phonon spectrum and lattice specific heat of the $HgBa_2$ CuO_4 high temperature superconductor, Physica C: Superconductivity **271** 1 (1996) 6-10.

[8] P. K. Jha, S.P. Sanyal, A lattice dynamical study of the role of pressure on Raman modes in high-T c $HgBa_2$ CuO_4, Physica C: Superconductivity **3** (1996) 259-262.

[9] P. K. Jha and S. P. Sanyal, Lattice vibrations in intermediate valence compounds SmS and TmSe, Indian Journal of Pure and Applied Physics **31** (1993) 469-473.