Journal of ELECTRONIC MATERIALS, Vol. 47, No. 7, 2018
https://doi.org/10.1007/s11664-018-6251-4

Ferromagnetic Phase Stability, Magnetic, Electronic, Elasto-Mechanical and Thermodynamic Properties of $BaCmO_3$ Perovskite Oxide

SAJAD AHMAD DAR,[1] VIPUL SRIVASTAVA,[2,5]
UMESH KUMAR SAKALLE,[3] and VANSHREE PAREY[4]

1.—Department of Physics, Govt. Motilal Vigyan Mahavidyalya College, Bhopal 462008, MP, India. 2.—Department of Physics, NRI Institute of Research & Technology, Bhopal 462021, MP, India. 3.—Department of Physics, S. N. P. G. College, Khandwa 450001, MP, India. 4.—Department of Physics, Barkatullah University, Bhopal 462026, MP, India. 5.—e-mail: vips73@yahoo.com

The structural, electronic, elasto-mechanical and thermodynamic properties of cubic ABO_3 perovskites $BaCmO_3$ has been successfully calculated within density functional theory via full potential linearized augmented plane wave. The structural study divulges ferromagnetic stability for the compound. For the precise calculation of electronic and magnetic properties a generalized gradient approximation (GGA), and a Hubbard approximation (GGA + U), (modified Becke Johnson approximation) mBJ have been incorporated. The electronic study portrays the half-metallic nature for the compound in all the approximations. The calculated magnetic moment with different approximations was found to be large and with an integer value of 6 μ_b, this integer value of magnetic moment also proves the half-metallic nature for $BaCmO_3$. The calculated elastic constants have been used to predict mechanical properties like the Young modulus (Y), the Shear modulus (G) and the Poisson ratio (v). The calculated B/G and Cauchy pressure (C_{12}-C_{44}) present the brittle nature for $BaCmO_3$. The thermodynamic parameters like heat capacity, thermal expansion, and Debye temperature have been calculated and examined in the temperature range of 0 K to 700 K and pressure between 0 GPa and 40 GPa. The melting temperature was also calculated and was found to be 1847 ± 300 K.

Key words: $BaCmO_3$, DFT, half-metallic and ferromagnetic, thermodynamics: elastic and mechanical properties

INTRODUCTION

Advances in material science and technology has led to an escalation in the search for novel materials due to mounting demands in different fields like ferromagnetism,[1] piezoelectricity,[2] ferroelectricity,[3] half-metallicity,[4,5] etc. For such wonderful demands, materials like perovskites and related compounds have always enjoyed a first place. Perovskite materials have found extensive applications in the novel device fabrications like gas sensing, sharp memory, thermoelectric devices, fuel cells and spintronics.[6–9]

Transuranic elements and their compounds have always remained a challenge for the experimentalist because of their radioactive nature. Advances in computational and theoretical methods have removed the barrier in handling these materials which are highly radioactive and has, hence, paved a way to investigate and predict the properties of these correlated and radio-active systems. Recently perovskites $BaAmO_3$, $SrPuO_3$,

---

(Received September 19, 2017; accepted March 21, 2018;

$BaPuO_3$ $SrAmO_3$[10–13] which contain transuranic elements at the B site have been reported for their electronic and thermo-physical properties. $BaCmO_3$, which is an important member of the perovskite family, has been reported to crystalize in cubic phase with space group Pm-3 m (221). The Curium-based compounds are potentially the important members of the perovskite family because of their correlated and highly complicated electronic structure. Not much is known about the electronic, mechanical and thermo-physical behavior of $BaCmO_3$ and in the literature we could only find its structure details, but, as far as its closely related compounds like $BaAmO_3$, $BaNpO_3$, $SrAmO_3$,[10–13] $BaThO_3$ $BaUO_3$, $SrUo_3$[14–16] are concerned, ample work has already been published. This evident lack of data on $BaCmO_3$ has motivated us to investigate this compound and to predict its properties.

In this paper we have made an attempt to discuss and evaluate the basic structural, electronic, magnetic, elasto-mechanical properties of $BaCmO_3$ in the framework of the most successful density functional theory (DFT),[17,18] using different exchange correlation potentials like GGA, GGA + U, mBJ.[19–21] For actinide element-based perovskite oxides, due importance has been given for thermodynamic investigations of these compounds,[22,23] and; hence, a Quasi harmonic Debye approximation[24–26] has been used for the prediction and evaluation of some basic thermodynamic parameters.

COMPUTATIONAL DETAILS

For the calculation of structural, electronic, elastic and magnetic properties, a full-potential linearized augmented plane wave (FP-LAPW)[27] method based on density functional theory (DFT)[17,18] as implemented in wien2 k code has been employed. The structural optimization has been attained within a generalized gradient approximation plus Hubbard approximation (GGA + U).[20] To further check the effect on our results, on-site modified Becke-Johnson (mBJ)[21] was also used for electronic and magnetic studies. In order to treat the f-electrons of Cm, GGA + U has been used. For the GGA + U approach, the density matrix was supposed to be diagonal and U and J are the same for all interactions. To include the U- term there are different methods,[28,29] here we have made use of the self-interaction correction method (SIC)[30] as implemented in wien2 k. The value of U_{eff} was varied from 2 eV to 8 eV and J was set to 0, so as to adjust the Cm-f in density of states. The results on electronic and magnetic calculations with the variation of U_{eff} produced similar results like half-metallicity and the integer value of the magnetic moment. The final U value was set to 5 eV. For energy convergence, $R_{\mathrm{MT}}K_{\mathrm{max}}$ was set to 7, where R_{MT} is the small atomic radius in the unit cell and K_{max} denotes the size of the largest **k** vector in the plane wave expansion. In the full potential arrangement the unit cell of the crystal is split into two different regions: (1) atomic spheres and (2) the interstitial region, and within the atomic sphere the wave function is extended in atomic-like functions (radial part times spherical harmonics) while in the interstitial area it is extended in a plane wave basis. Inside the sphere the $L_{\mathrm{max}} = 10$, while the charge density is Fourier expanded up to $G_{\mathrm{max}} = 12$ $(\mathrm{a.u.})^{-1}$. The self-consistent calculations are converged when the total energy of the system is stable within 10^{-4} Ry. A dense mesh of 1500 K points and the tetrahedral method[31] have been used for the brillouin zone integration.

The calculations of elastic constants require familiarity of the derivative of the energy as a function of the lattice tension. The balance of the cubic lattice is as such that it reduces the 21 dependent elastic constants to three independent elastic constants, namely C_{11}, C_{12} and C_{44}. The elastic stability criteria for a cubic crystal under ambient conditions are $C_{11} + 2C_{12} > 0$, $C_{44} > 0$, $C_{11} - C_{12} > 0$ and $C_{12} < B < C_{11}$. The elastic constants have been calculated within GGA and GGA + U by the method developed by Charpin as integrated in the wien2 k package.[32]

For thermodynamic calculations the quasi-harmonic Debye model[24–26] has been implemented for temperature and pressure dependence of specific heat at constant volume (C_{V}), unit cell volume and Debye temperature. The optimized Birch-Murnagan's[33] data generated from GGA + U calculations has been used as input for the quasi-harmonic Debye model. The thermodynamic quantities remained the same within GGA and GGA + U.

RESULTS AND DISCUSSION

Structural Properties

$BaCmO_3$ perovskite has been reported in cubic phase with a lattice constant of 4.364 Å.[34] The Ba atoms are located at corners (0, 0, 0), Cm at center (0.5, 0.5, 0.5) and O atoms are sited at face centers (0.5, 0.5, 0), (0.5, 0, 0.5), (0, 0.5, 0.5) of cubic unit cell. The geometry and structural stuffs for cubic $BaCmO_3$ have been calculated using Birch-Murnaghan's[33] equation of state by appropriate fitting of total energy as a function of unit cell volume in ferromagnetic (FM), paramagnetic (PM) and antiferromagnetic (AFM) cases within GGA + U. The ground state energy establishes a lowest value for the ferromagnetic phase as presented in Fig. 1, thus a stable state. The ground state parameters like bulk modulus, lattice constant and pressure derivatives are grouped in Table I within GGA and GGA + U.

Further, we have designed the lattice constant for $BaCmO_3$ analytically, from the information of ionic radius of the individual elements using Eq. 1.[35]

$$a_0 = \alpha + \beta(r_{Ba} + r_O) + \gamma(r_{Cm} + r_O), \quad (1)$$

where α, β, γ are constants whose values are 0.06741, 0.4905 and 1.2921, respectively, and the ionic radii are r_{Ba}= (1.61), r_{Cm}= (0.85) and r_O= (1.35).[36] The experimental lattice constant and that obtained by analytical technique and also the one calculated from DFT show a close similitude. The tolerance factor, which is an important constraint to account for perovskite compound symmetry, has also been designed by the well-known Goldschmidt's formula[37] from ionic radius data, and has also been calculated from the bound length data for $BaCmO_3$.

$$t = \frac{0.707(r_{Ba} + r_O)}{(r_{Cm} + r_O)} \quad (2)$$

$$t = \frac{0.707(\mathrm{Ba} - \mathrm{O})}{(\mathrm{Cm} - \mathrm{O})} \quad (3)$$

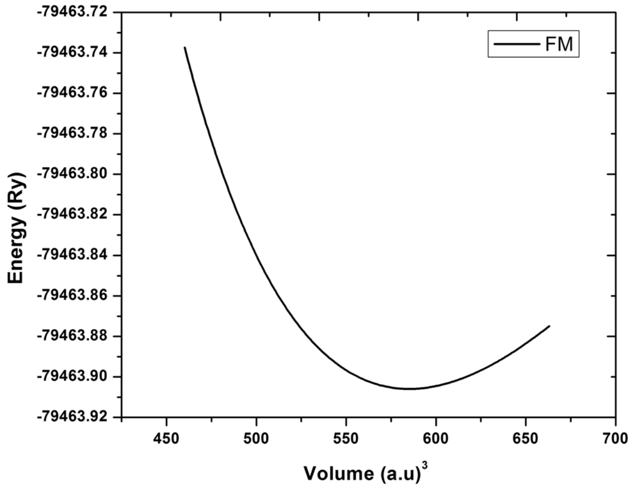

Fig. 1. Energy as a function of volume for $BaCmO_3$ with GGA + *U*.

In Eq. 2, Ba – O and Cm – O are the average bound length's between Ba-O and Cm-O. The calculated values of tolerance factor from both Goldschmidt's formula and bond length data properly follow the criteria for cubic symmetry (0.93–1.04)[38,39] and are grouped in Table I.

Electronic and Magnetic Properties

In density functional theory electronic properties are appropriately represented by density of states and band structure results. Figure 2a represents combined total density of states (TDOS) within different correlation potentials like GGA, GGA + *U* and mBJ. From this figure, it is clearly observed that the density of state that results with different approximations is almost similar, presenting 100% of spin polarization at the Fermi level. The Fermi level is set at 0 eV, separating the conduction band from the the valance band. For spinup states the Fermi-level remains completely occupied presenting the metallic nature for the compound and for spin down states the Fermi-level falls in a gap resulting in a semi-conducting nature for the compound. Thus, the overall TDOS presents a half-metallic nature for the compound. The verification of these results is also explained by PDOS as depicted in Fig. 2b. The PDOS has been plotted using GGA + *U* for Ba-d, f, Cm d, f and O-s, p states. From this figure it is clear that the metallic nature in spinup states for the compound is due to the Cm-f and O-p states hybridized with one another and in case of spindown states the f- states of Cm are pulled inside the conduction band and O-p states are pulled towards the valence band, thereby generating a gap in spindown states. In spinup states the Cm-f states are scattered from – 4 eV inside the valance band to 1.1 eV ithe n conduction band having maximum density at – 4.2 eV and for spi-n down states these Cm-f states are scattered from 4 eV to 6.2 eV in the conduction band enjoying the maximum density at 6 eV. Thus, the TDOS and PDOS results both display a half-metallic nature for $BaCmO_3$.

Table I. Calculated value of lattice constant (a_0), bulk modulus (B_0), pressure derivative (B'), tolerance factor (t), and energy (E_0 in Ry) at equilibrium lattice constant

$BaCmO_3$	GGA	GGA + *U*	Exp.	Ionic radius method
a_0 (Å)	4.425	4.4261	4.363[34]	4.49
B (GPa)	113.85	113.55		
B'	5.026	5.111		
E_0	– 79,463.9045	– 79,643.9059		
t	0.99	0.99		0.95
Bond Length				
Ba–O (Å)	3.23	3.23		
Ba–Cm (Å)	3.955	3.955		
Cm-O (Å)	2.283	2.283		

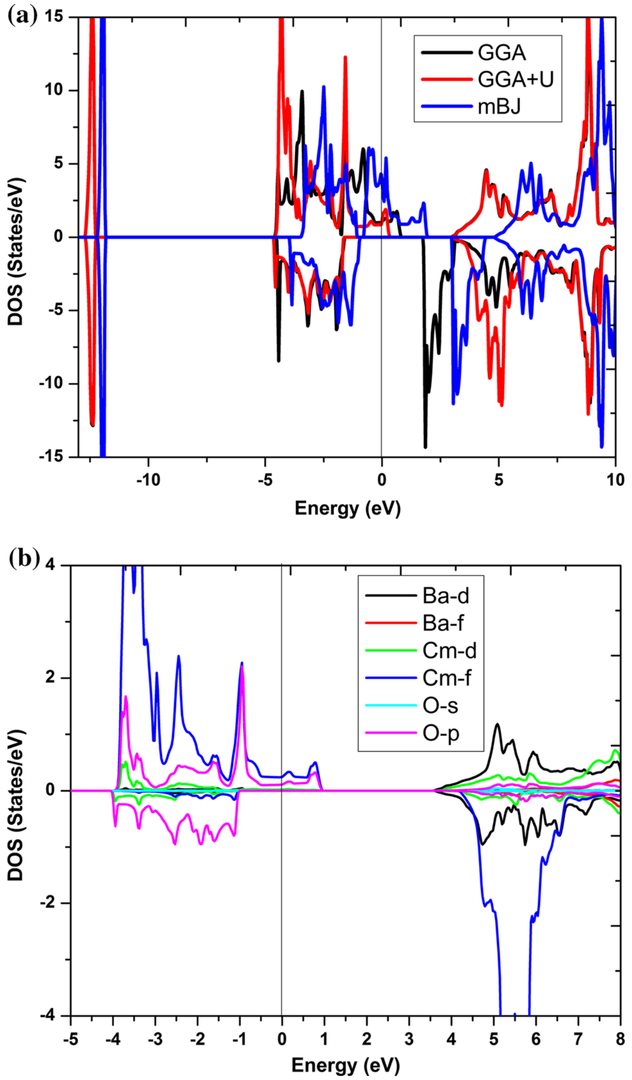

Fig. 2. (a, b) Total and partial density of states for spinup and spindown states for $BaCmO_3$.

The band structure results are depicted in Fig. S1a–c (see supplementary data file) the band structure results have been plotted within GGA, mBJ and GGA + *U*. From the band picture it is clear that the value of band gap in case of spin down states increases as we go from GGA < mBJ < GGA + *U*. The band gap values of 3.33 eV, 3.92 eV and 4.49 eV were found respectively within GGA, mBJ and GGA + *U*. The complete band profile presents the half-metallic nature for the compound.

The total and partial magnetic moments for $BaCmO_3$ have been obtained with GGA, GGA + *U* and mBJ. The magnetic contribution in materials is a result of the summation of the partial moments of individual elements and the interstitial moments. The total magnetic moment obtained in all the three approximations used has a large and integer value of 6 μ_B shown in Table II. The magnetism in this compound is mainly due to the Cm element as it is the main contributor to the total moment. The partial moment of the Cm element shows a great variation on the application of Hubbard *U* and mBJ potentials. The value of partial moment of Cm is 5.969 μ_B, 6.38 μ_B and 6.01 μ_B respectively, for GGA, GGA + *U* and mBJ. Hence, it is clear that the ferromagnetic nature and large value of total magnetic moment for $BaCmO_3$ is mainly due to Cm. The values of interstitial, partial and total magnetic moments are presented in Table II. Thus, the large magnetic moment and its integer value further elucidate the half-metallic[15] and ferromagnetic nature for $BaCmO_3$.

For the estimation of the Curie temperature, we have engaged Eq. 4, within the bounds of the Heisenberg model.[40]

$$T_C = \frac{\Delta E}{3k_B}, \tag{4}$$

where k_B is the Boltzman constant and ΔE is the energy difference between non- magnetic and ferromagnetic phase. The value of the Curie temperature was found to be 1067 K, which is larger than the room temperature and, hence, can find applications in magneto-electronic and spintronics devices.[40]

Elastic and Mechanical Properties

The elastic constant calculations help to know the ability of a material to deform on the application of force and further help in the estimation of the stability of a material. The valuation of elastic constants is a vital procedure in determining the mechanical stability, nature of bounding forces, ductility and various thermodynamic quantities like Debye temperature, specific heat, and melting temperature. The elastic constant values C_{ij} (C_{11}, C_{12}, C_{44}) were estimated from the relation of strain as a function of volume[41,42] and tabulated in Table III. Several theoretical models have so far been developed for the precise calculation of elastic constants. In this paper, the Charpin method[31] as implemented in wien2 k code has been employed for the determination of these elastic constants C_{ij} (C_{11}, C_{12}, C_{44}). We have calculated the elastic constants in the case of GGA and GGA + *U*. For crystals having cubic symmetry, the stability criteria are given as[43];

$$(C_{11} - C_{12}) > 0$$

$$C_{11} > 0, C_{44} > 0$$

$$(C_{11} + 2C_{12}) > 0$$

$$C_{12} < B < C_{11}$$

The abovementioned standards are properly followed by the calculated values of elastic constants

Table II. Calculated magnetic moment for ferromagnetic $BaCmO_3$ within GGA, GGA + *U* and mBJ (in bohrmagneton μ_B)

Compound	Configuration	M_{int}	M_{Ba}	M_{Cm}	M_O	M_{Tot}
$BaCmO_3$	GGA	0.02058	0.00763	5.96946	− 0.06094	6.00
	GGA + *U*	0.14487	0.00841	6.38473	− 0.17931	6.00
	mBJ	0.12466	0.00411	6.01049	− 0.04638	6.00

Table III. Calculated elastic constants C_{11}, C_{12}, and C_{44} in (GPa) and Bulk Modulus *B* (GPa); Shear Modulus *G* (GPa); Young's modulus *Y* (GPa); Poisson's ratio *v*; Zener anisotropy factor *A*; *B*/*G* ratio; Cauchy pressure C_{12}-C_{44}, density ρ (g/cm^3); longitudinal, transverse, and average sound velocity (v_l, v_t, v_m respectively, in m/s); melting temperature T_m (K); and Debye temperature (θ_D in K) for $BaCmO_3$

$BaCmO_3$	GGA	GGA + *U*	$BaAmO_3$[11]
C_{11}	219	220.65	220.18
C_{12}	60.37	60.15	67.53
C_{44}	48.67	52.18	46.59
B	113.78	113.65	119
G	59.24	62.03	58.49
Y	155.54	157.48	150.63
v	0.2721	0.2703	0.28
B/G	1.92	1.8321	2.02
C_{12}-C_{44}	11.7	7.97	20.93
A	0.61	0.65	0.61
ρ	8.28	8.27	8.261
V_l	4825.03	4872.70	4898
V_t	2674.80	2738.723	2668
V_m	2978.712	3038.346	2976
T_m	1847 ± 300	1857 ± 300	–
θ_D	342.39	354.16	342

and have been presented in (Table III). The mechanical properties like Young's modulus (*E*), which deals with the physical toughness of the material, Poisson's ratio (*v*) that explains the nature of the bonding forces, Bulk modulus (*B*) which delivers a sign about material stiffness, and Shear modulus (*G*) as an indicator of plastic twist of the materials have been calculated from elastic constant values (C_{11}, C_{12}, C_{44}) using the Voigt-Reuss-Hill approximation[44,45] and presented in Table III.

$$G_V = \frac{1}{5}(C_{11} - C_{12} + 3C_{44}) \tag{5}$$

$$G_R = \frac{5(C_{11} - C_{12})C_{44}}{3(C_{11} - C_{12}) + 4C_{44}} \tag{6}$$

$$G = \frac{G_V + G_R}{2} \tag{7}$$

$$Y = \frac{9BG}{(3B + G)} \tag{8}$$

$$v = \frac{3B - 2G}{2(3B + G)}, \tag{9}$$

where *B* is the Bulk modulus, G_V and G_R are Voigt's and Reuss's Shear moduli.

Anisotropy denoted by *A* is an important bound that describes the distinctive properties such as electronic and magnetic properties in different directions of its structure. According to this bound, a material is isotropic, if the value of the *A* factor is less or equal to unity or otherwise anisotropic. The value of anisotropy is calculated by[46];

$$A = \frac{2C_{44}}{C_{11} - C_{12}}. \tag{10}$$

The calculated value of *A* for $BaCmO_3$ is equal to 0.61, 0.65, respectively, within GGA and GGA + *U*, hence, less than unity, and thus will show anisotropic nature.

Poisson's ratio (*v*) describes the variety of bonding forces between the atoms. The assortment of Poisson's ratio is 0.25–0.50[47,48] for the materials displaying central forces or otherwise directional. For materials having covalent bonding the (v) take the value of 0.1, for ionic materials it is 0.25 and for metallic materials it is 0.33. Our calculated value of (v) $BaCmO_3$ is 0.27 both GGA and GGA + U, which lies in between 0.25 and 0.33 and, hence, suggests a mixture of ionic and metallic bounding. The B/G ratio offers the evidence on ductility and brittleness of a material. By Pugh,[49] a solid behaves as brittle if the B/G ratio $<$ 1.75 and ductile the if B/G ratio $>$ 1.75. The calculated value the of B/G ratio was 1.92 and 1.83, respectively, within GGA and GGA + U and, hence, higher than the limit value of 1.75, and thus will show a ductile nature. Further, the Cauchy pressure (C_{12}-C_{44}) offers the criteria for the ductility and brittleness of a material. Its positive value characterizes a material as ductile and a negative value as brittle. The calculated value was found to be positive and, hence, $BaCmO_3$ will show a ductile nature as discussed above.

Debye temperature, θ_D helps to elucidate specific presentation of the solids-like performance of heat capacity and thermal expansion and also provides the information about the features of a material under the influence of temperature and pressure. One of the classic approaches to find Debye temperature is obtained from the average sound velocity, v_m by the following equation[50]

$$\theta_D = \frac{h}{k_B}\left[\frac{3}{4\pi V_a}\right]^{1/3} v_m, \tag{11}$$

where h is Plank's constant, K_B is Boltzmann's constant and V_a is the average atomic volume, v_m average wave velocity, given by the following relation:

$$v_m = \left[\frac{1}{3}\left(\frac{2}{v_t^3} + \frac{1}{v_l^3}\right)\right]^{-\frac{1}{3}}. \tag{12}$$

Where v_l and v_t are longitudinal and transverse elastic wave velocities and determined by the following relations[50]:

$$v_t = \left(\frac{G}{\rho}\right)^{\frac{1}{2}}, \tag{13}$$

$$v_l = \left(\frac{3B + 4G}{3\rho}\right)^{\frac{1}{2}}. \tag{14}$$

The predicted values of Debye temperature for $BaCmO_3$ from the elastic data is 342.39 K and 354 K, respectively, within GGA and GGA + U. The values of elastic constants have also been employed to predict another essential thermodynamic factor called melting temperature[51];

$$T_m(K) = [553(K) + (5.911)C_{12}]\text{GPa} \pm 300\,\text{K}. \tag{15}$$

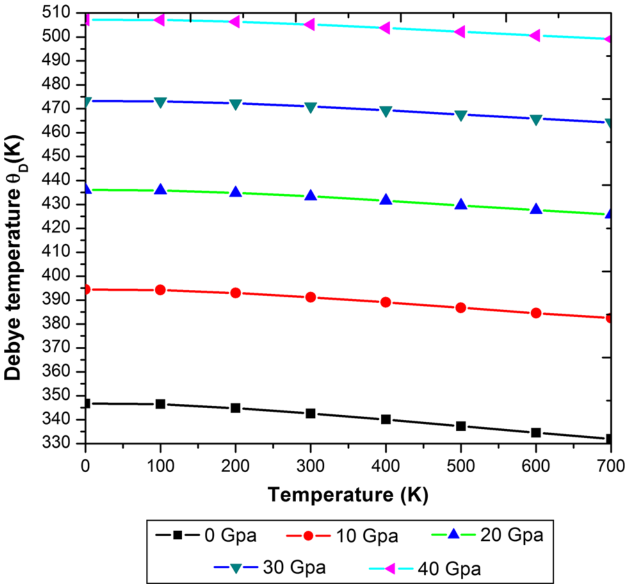

Fig. 3. Debye temperature (θ_D) as a function of temperature and pressure for $BaCmO_3$.

All the calculated values of elastic constants, mechanical and thermodynamic properties are grouped in Table III within GGA and GGA + U and a comparison of our results has been made with the closely related compound $BaAmO_3$.

Thermodynamic Properties

For the investigation of thermodynamic parameters, the quasi-harmonic Debye approximation[23–25] has been employed to check the temperature and pressure dependence of important thermodynamic parameters like specific heat at constant volume (C_v), the Grüneisen parameter (γ), and the Debye temperature (θ_D). The variation in temperature has been done from 0 K to 700 K and pressure has been varied from 0 GPa to 40 GPa because the quasi harmonic Debye model remains completely valid in the temperature range of 0 K to 1000 K.

The Debye temperature variation with respect to temperature/pressure is presented in Fig. 3. From this figure it is clear that the Debye temperature shows a slight decreasing trend as the temperature is increased at a particular pressure and increases with pressure at a particular temperature. The obtained value of Debye temperature at 0 K and 0 GPa from the quasi harmonic approximation and that from the classical model show almost a close resemblance.

The Grüneisen parameter (γ) is also an important thermodynamic quantity that describes the change in vibrational frequency of a lattice when the material is exposed to temperature and pressure variation.[52] The temperature and pressure

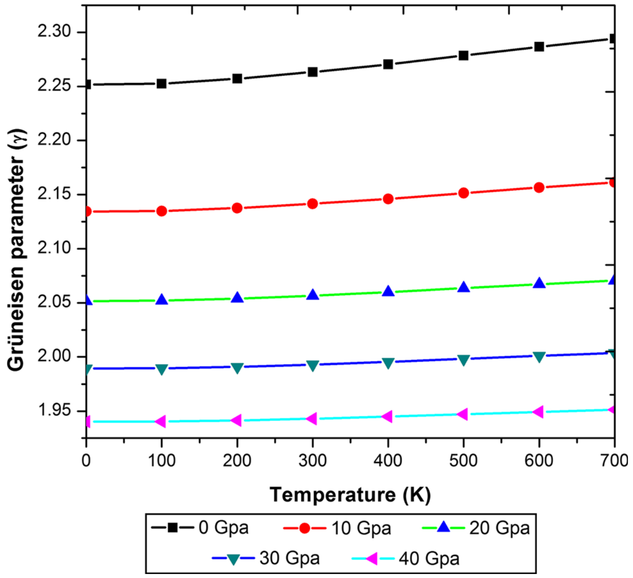

Fig. 4. Variation of Grüneisen parameter (γ), as a function of temperature and pressure for $BaCmO_3$.

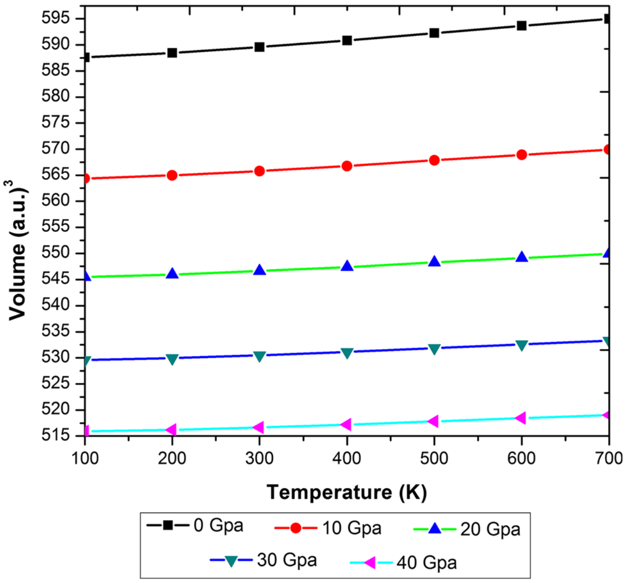

Fig. 5. Variation of unit cell volume as a function of temperature and pressure for $BaCmO_3$.

dependence of (γ) for $BaCmO_3$ is plotted in Fig. 4. The value of (γ) increases slowly with increasing temperature at constant pressure but pressure has a reverse effect, (γ) decreases with increasing pressure. The calculated value of (γ) at 0 K and 0 GPa of pressure is 1.9471.

The pressure and temperature dependence of volume for $BaCmO_3$ is illustrated in Fig. 5. From this figure it is clear that an increasing trend in volume is observed with increasing temperature, while on the other hand, a decrease in volume is observed as the pressure is increased. This volume change with increasing temperature and pressure is practically a common trend in solids. The effect of temperature on volume is not so much as compared to pressure. Further, we have computed specific heat at constant volume (C_V) over a temperature and pressure range of 0 K to 700 K and 0 GPa to 40 GPa, respectively, as presented in Fig. 6. One can see from the figure that C_V increases rapidly under the lower temperature range of 0 K to 300 K, but above 300 K a slow increase in C_V can be observed, which further becomes constant at a temperature of 700 K and reaches the Dulong- Petit limit.[53] The calculated value of C_V for $BaCmO_3$ at 300 K was found to be 108.37 J mol^{-1} K. Since in the literature we could not find the comparison for the elastic and thermodynamic study, but the similar compound with actinide-based Americium $BaAmO_3$ and $SrAmO_3$[10,11] have almost similar results.

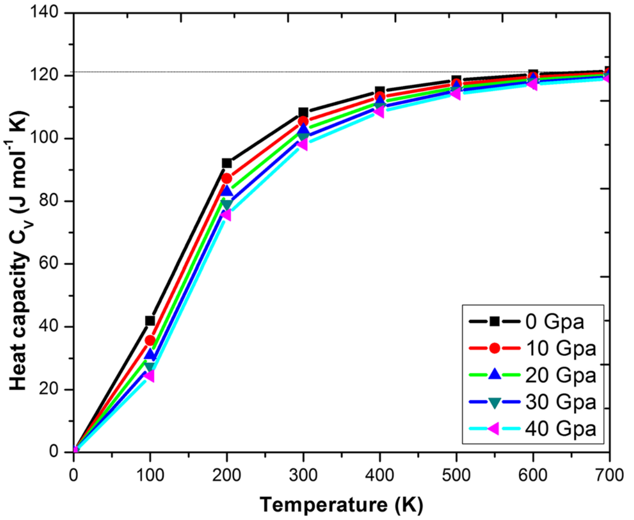

Fig. 6. Variation of specific heat at constant volume (C_V) with temperature and pressure for $BaCmO_3$.

CONCLUSION

We have presented successful ab-intio calculations based upon density functional theory for the ferromagnetic $BaCmO_3$ perovskite oxide. The material display of a half-metallic nature for the combined spins with the metallic in spinup channels and the semi-conducting for spindown channels. The ferromagnetic phase stability with a large magnetic moment of 6 μ_B implies that the compound may be used for spintronics, magnetic devices and can further find its application for direct band gap semi-conductors. The elastic constants for the compound have been predicted for the first time. The mechanical profile for the compound shows a ductile and an anisotropic nature. The thermodynamic properties have also been for the first time calculated for $BaCmO_3$.

ACKNOWLEDGEMENT

The authors gratefully acknowledge Dr. Gitanali Pagare for computational help and support, further author Vipul Srivastava, acknowledge MPCST for the grant of project.

ELECTRONIC SUPPLEMENTARY MATERIAL

The online version of this article (https://doi.org/10.1007/s11664-018-6251-4) contains supplementary material, which is available to authorized users.

REFERENCES

1. M. Imada, A. Fujimori, and Y. Tokura, *Mod. Phys.* 70, 1039 (1998).
2. F.S. Hickernell, *IEEE Trans. Ultrason.* 52, 737 (2005).
3. P. Zubko, S. Gariglio, M. Gabay, P. Ghosez, and J.M. Triscone, *Annu. Rev. Condens. Matter Phys.* 2, 141 (2011).
4. A.J. Millis, B.I. Shraiman, and R. Muller, *Phys. Rev. Lett.* 77, 175 (1996).
5. Y. Tokura, eds., *Advances in condensed matter science*, Vol. 2 (The Netherlands: Gordan and Breach, 2000).
6. M. Bibes and A. Barthélémy, *Nat. Mater.* 7, 425 (2008).
7. N.C. Bristowe, J. Varignon, D. Fontaine, E. Bousquet, and P. Ghosez, *Nat. Commun.* 6, 6677 (2015).
8. J.F. Scott, *Nat. Mater.* 6, 256 (2007).
9. Y. Tokura and N. Nagaosa, *Science* 288, 462 (2000).
10. S.A. Dar, V. Srivastava, and U.K. Sakalle, *J. Supercond. Nov. Magn.* 30, 3055 (2017).
11. S.A. Dar, V. Srivastava, U.K. Sakalle, S.A. Khandy, and D.C. Gupta, *J. Supercond. Nov. Magn.* 31, 141 (2018).
12. S.A. Dar, V. Srivastava, U.K. Sakalle, and G. Pagare, *J. Supercond. Nov. Magn*. (2018). https://doi.org/10.1007/s10948-018-4574-2.
13. S.A. Dar, V. Srivastava, U.K. Sakalle, A. Rashid, and G. Pagare, *Mater. Res. Express* 5, 026106 (2018).
14. Z. Ali, I. Ahmad, B. Amin, J. Maqsood, A. Afaq, M. Maqbool, I. Khan, and M. Zahid, *Opt. Mat.* 33, 553 (2011).
15. Z. Ali, I. Ahmad, and A.H. Reshak, *Phys. B* 410, 217 (2013).
16. B. Sahli, H. Bouafia, B. Abidri, A. Abdellaoui, S. Hiadsi, A. Akriche, N. Benkhettou, and D. Rached, *J Alloys Compd.* 635, 163 (2015).
17. P. Blaha, K. Schwarz, G.K.H. Madsen, D. Kuasnicke, and J. Luitz, *Introduction to WIEN2 K, An Augmented plane wave plus local orbitals program for calculating crystal properties* (Vienna: Vienna University of Technology, 2001).
18. K. Schwarz, P. Blaha, and G.K.H. Madsen, *Comp. Phys. Commun.* 147, 71 (2002).
19. J.P. Perdew, K. Burke, and M. Ernzerhof, *Phys. Rev. Lett.* 77, 3865 (1996).
20. S.A. Dar, S.A. Khandy, I. Islam, D.C. Gupta, U.K. Sakalle, V. Srivastava, and K. Parray, *Chin. J. Phys.* 55, 1769 (2017).
21. F. Tran and P. Blaha, *Phys. Rev. Lett.* 102, 226401 (2009).
22. K. Tanaka, I. Sato, T. Hirosawa, K. Kurosaki, H. Muta, and S. Yamanaka, *J. Nucl. Mater.* 422, 163 (2012).
23. K. Tanaka, I. Sato, T. Hirosawa, K. Kurosaki, H. Muta, and S. Yamanaka, *J. Nucl. Mater.* 414, 316 (2011).
24. M.A. Blanco, A.M. Pendas, and E.J. Francisco, *J. Mol. Struct. Theochem.* 268, 245 (1996).
25. A. Otero-de-la-Roza, D. Abbasi-Pérez, and V. Luaña, *Comput. Phys. Commun.* 182, 2232 (2011).
26. A. Otero-de-la-Roza and V. Luaña, *Phys. Rev. B* 84, 184103 (2011).
27. Z. Wu and R.E. Cohen, *Phys. Rev. B* 73, 235116 (2006).
28. A.G. Petukhov and I.I. Mazin, *Phys. Rev. B* 67, 153106 (2003).
29. P. Novak, J. Kunes, L. Chaput, and W.E. Pickett, *Phys. Status Solidi B* 243, 563 (2006).
30. V.I. Aisimov, I.V. Solovye, M.A. Korotin, M.T. Czyzyk, and G.A. Sawatzky, *Phys. Rev. B* 48, 16929 (1993).
31. H.J. Monkhorst and J.D. Pack, *Phys. Rev. B* 13, 5188 (1976).
32. T. Charpin, A Package for Calculating elastic tensors of cubic phases using WIEN: Laboratory of Geometrix F-75252 (Paris, France) (2001).
33. F. Birch, *J. Appl. Phys.* 9, 279 (1938).
34. J. Fuger, R.G. Haire, and J.R. Peterson, *J. Alloys Compd.* 200, 181 (1993).
35. R. Ubic, *J. Am. Ceram. Soc.* 90, 3326 (2007).
36. R.D. Shannon, Acta Crystallogr. *Sect. A: Cryst. Phys. Diffr. Theor. Gen. Crystallogr.* 32, 751 (1976).
37. J.B. Goodenogh, *Rep. Prog. Phys.* 67, 1915 (2004).
38. L.E. Russel, D.L. Harrison, and N.H. Brett, *J. Nucl. Mater.* 2, 310 (1960).
39. N. Xu, H. Zhao, X. Zhou, W. Wei, X. Lu, W. Ding, and F. Li, *Int. J. Hydrog. Energy* 35, 7295 (2010).
40. P.L. Yan, J.M. Zhang, B. Zhou, and K.W. Xu, *J. Phys. D:Appl. Phys.* 49, 255002 (2016).
41. S.A. Dar, V. Srivastava, and U.K. Sakalle, *Mater. Res. Express* 4, 086304 (2017).
42. S.A. Dar, V. Srivastava, and U.K. Sakalle, *J. Electron. Mater.* 46, 6870 (2017).
43. G.V. Sinko and N.A. Smirnov, *J. Phys. Condens. Matter* 14, 6989 (2002).
44. R. Hill, *Proc. Phy. Soc. London* 65, 349 (1952).
45. A. Reuss and Z. Angew, *Mater. Phys.* 9, 49 (1929).
46. V. Tvergaard and J.W. Hirtchinson, *J. Am. Ceram. Soc.* 71, 157 (1988).
47. D.G. Pertifor, *Mater. Sci. Technol.* 8, 345 (1992).
48. J. Haines, J.M. Leger, and G. Bocquillon, *Ann. Rev. Mater. Sci.* 31, 1 (2001).
49. S.F. Pugh, *Philos. Mag.* 45, 823 (1954).
50. E. Schreiber, O.L. Anderson, and N. Soga, *Elastic constants and measurements* (New York: M.C Graw Hill, 1973).
51. K. Bencherif, A. Yakoubi, N. Della, O.M. Abid, H. Khachai, and R. Ahmad, et al., *J. Electr. Mater.* 45, 3479 (2016).
52. L. Quiang, H. Duo-Hui, C. Qi-Long, and W. Fan-Hou, *Chin. Phys. B* 22, 037101 (2013).
53. A.T. Petit and P.L. Dulong, *Ann. Chim. Phys.* 10, 395 (1819).