Journal of Nano- and Electronic Physics
Vol. **12** No 2, 02031(4pp) (2020)

Журнал нано- та електронної фізики
Том **12** № 2, 02031(4cc) (2020)

Ground State Stability and Thermal Properties of ErCu Using First Principles Study

Dhara Raval[1], Bindiya Babariya[1], Sanjeev K. Gupta[2], P. N. Gajjar[1,*]

[1] *Department of Physics, University School of Sciences, Gujarat University, 380009 Ahmedabad, India*
[2] *Computational Materials and Nanoscience Group, Department of Physics, St. Xavier's College, 380009 Ahmedabad, India*

(Received 18 February 2020; revised manuscript received 15 April 2020; published online 25 April 2020)

We have investigated elastic, vibrational and thermal properties of B_2 type ErCu intermetallic compound using density functional theory (DFT). The positive phonon frequencies reflect the dynamical stability of ErCu intermetallic compound in the B_2 type cubic structure phase. Furthermore, the density functional perturbation theory (DFPT) as implemented in quasi-harmonic approximation (QHA) was used for the calculation of thermal properties such as vibrational energy ΔF, entropy S, internal energy ΔE and constant-volume specific heat Cv of the ErCu. The entropy of ErCu is ~ 18 $J \cdot K^{-1} \cdot mol^{-1}$ that concluded that, the ErCu compound is not harder compound. The computed Poisson's ratio (σ), Young's modulus (E), bulk modulus (B) and shear modulus (GH) are 0.30, 66.65 GPa, 62.99 GPa and 25.18 GPa respectively. The B/G_H ratio is 2.50, which confirmed the good ductility of ErCu intermetallic compound.

Keywords: ErCu, Density Functional Theory, Elastic properties, Thermal properties.

DOI: 10.21272/jnep.12(2).02031 PACS numbers: 46.15. – x, 0.270. – c, 61.50 – f, 62.30 + d, 63.20 – e, 65.40 – b

1. INTRODUCTION

The intermetallic compounds received much attention due to their superior physical, electrical, magnetic, mechanical and chemical properties [1-7]. It is well know that at elevated temperature, the intermetallic compounds have capacity to improve their performance in engineering applications. Owing to their high ductility, oxidation resistance, high tensile strength, stiffness and low density; they are used in aerospace industry [2, 8]. The partially filled '*f* electrons of Er show the ErCu holds extraordinarily high ductility and crystallizes in the CsCl type cubic structure [9, 10]. Few stoichiometry of ErCu intermetallic compounds have been studied experimentally and theoretically with CsCl type structure [2, 9-16]. To best of our knowledge, there were no experimental and theoretical results for the comparison of vibrational and thermal properties of ErCu. Therefore, we have investigated vibrational and thermal properties of ErCu and explored phonon dispersive curve, phonon density of states (PDOS) and thermal properties such as vibrational energy ΔF, entropy S, internal energy ΔE and constant-volume specific heat C_v. Moreover, the elastic properties viz; bulk modulus B, shear modulus GH, Young's modulus E, Poisson's ratio σ, Pugh's ratio (B/GH) and elastic constants (C_{11}, C_{12} and C_{44}) of ErCu compound have been also investigated.

2. COMPUTATIONAL METHOD

The present study was carried out using density functional perturbation theory (DFPT) formalism with Troullier Martin type pseudopotential [17-18] for Er and ultrasoft exchange and correlation pseudopotential for Cu [19-23]. The qausi harmonic approximation (QHA) code developed by the Baroni et al. is used to investigate the thermal properties [24]. All calculation is explored with two atom basis located, where Er atom at (0.5, 0.5, 0.5) and Cu atom at (0.0, 0.0, 0.0) with cutoff energy 370 Ry and 16×16×16 Monk horst-pack grid [25]. Phonon code is used to find the vibrational and thermal properties of ErCu intermatallic compound using the Quantum Espresso code [26, 27]. The vibrational properties have been obtained from optimized lattice parameter of ErCu intermatallic compound with spin-polarized case [28]. The phonon frequency spectra were studies along the high symmetry points Γ - X - M - Γ- R - X [29].

3. RESULTS AND DISCUSSION

In our previous work [27], we already optimized the geometrically stable lattice constant $a_0 = 3.414$ Å of ErCu B_2 type structure and based on the stability of system. Moreover, we had also appraised the electronic properties such as band structure, density of States, partial density of states, charge density and Fermi surface of ErCu for majority and minority spin cases. Hence, the same lattice constant of ErCu was used for further study.

3.1 Vibrational Properties

The calculated phonon dispersion relation of ErCu having two atoms in the system, the phonon dispersion curve has total six branches as shown in Fig. 1. The span of one LA (longitudinal acoustic), one LO (longitudinal optical), two TA (transverse acoustic) and two TO (transverse optical) is within the frequency 140 cm^{-1} range. The positive phonon frequencies reflect the dynamical stability of the ErCu in B2 phase. At the frequency of 50 cm^{-1}, LA, TA and LO branches were overlapping at the M-point and near the X-point and the LA and LO branches are overlapping at the 101 cm^{-1} frequency. It is noticed that one optical and two acoustic branches are triply degenerate at the Γ-points that reveal the metallic nature of ErCu.

* pngajjar@gujaratuniversity.ac.in

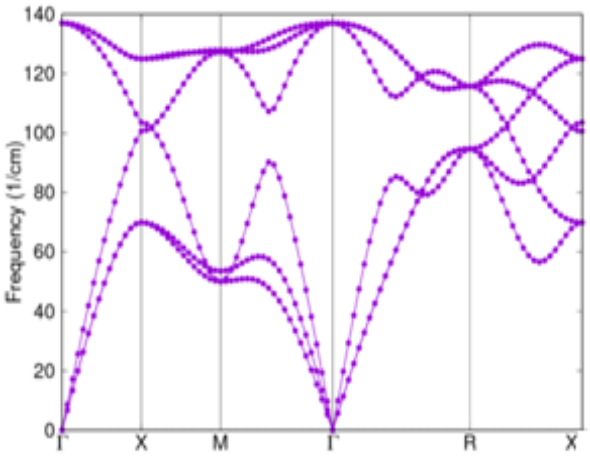

Fig. 1 – Phonon dispersion curves along the high symmetry direction in B_2 type ErCu

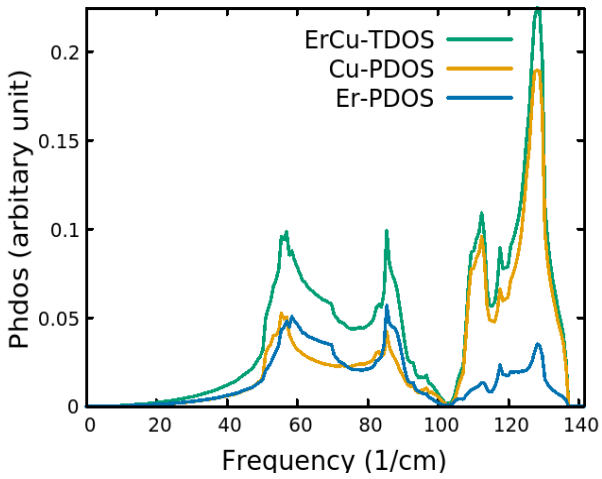

Fig. 2 – Total and partial phonon density of states of ErCu in cubic phase along the high symmetry directions

Table 1 – Calculated bulk modulus B, Young's modulus E, shear modulus G_H, Poission Ratio σ, Pugh's constant B/GH and elastic constants C_{11}, C_{12},C_{44} and comparison of other available data

Sr. No	Property	Present calculation	Other calculation
1	Bulk Modulus B (GPa)	62.99	63.14 [10], 76.62 [2]
2	Yong Modulus E (GPa)	66.65	79.97 [10], 96.03 [2]
3	Shear Modulus GH (GPa)	25.18	30.84 [10], 36.64 [2]
4	Poisson Ratio σ	0.30	0.29 [10], 0.31 [2]
5	Pugh's ratio (B/G_H)	2.50	2.12 [10], 2.30 [2]
6	Elastic Constant C_{11} (GPa)	85.07	157.23 [10], 129.71 [2]
7	Elastic Constant C_{12} (GPa)	51.95	19.60 [10], 61.77 [2]
8	Elastic Constant C_{44} (GPa)	38.06	16.8 [10], 38.54 [2]

The total and partial phonon density of states of ErCu is shown in Fig. 2. In partial phonon DOS of Er atom has two major peaks one at 58.61 cm^{-1} and second at 85.73 cm^{-1} frequency. While, in partial phonon DOS of Cu atom contribution leads four successive peaks at the 56.07 cm^{-1}, 86.01 cm^{-1}, 112.57 cm^{-1} and 128.39 cm^{-1} successively. Among them first peak arises due to flat curve of the acoustics mode frequency at the 57.20 cm^{-1}, second peak appeared due to the overlapping of the LO and TO modes at the R-point with frequency 85.73 cm^{-1}, third and fourth peaks are resulted from the highly overlapping of LA and TO modes at R-point to X point at 112.57 cm^{-1} and 128.67 cm^{-1} respectively.

3.2 Elastic Properties

The elastic constants are important parameters to study elastic properties of the system. Moreover, elastic constants are requisite parameters that provide the information about the structural stabilities, ductility, inter-atomic forces and stiffness of the materials. The bulk modulus B (GPa) represents the resistance to fracture while shear modulus G_H (GPa) represents the resistance to plastic deformation. In cubic crystals, there are only three independent elastic constant C_{11}, C_{12} and C_{44}. The bulk modulus B, Shear modulus G_H, Young's modulus E, Poisson's ratio σ, Pugh's ratio (B/G_H) and elastic constants (C_{11}, C_{12} and C_{44}) are tabulated in Table 1.

The mechanical stability of the ErCu cubic crystal is satisfied by Born-Huang stability criteria: C_{11}-$C_{12} > 0$, $C_{11} > 0$, $C_{44} > 0$ and $(C_{11} + 2C_{12}) > 0$ [30]. Our calculated elastic constants of ErCu follow cubic stability conditions $C_{12} < B < C_{11}$. Which clearly indicate the stability of the ErCu compound in B_2 cubic phase. It is also found that calculated values are in reasonable agreement with available other results [2, 10]. According to Pugh's criteria material is brittle when, $B/G_H > 1.75$ or ductile $B/G_H < 1.75$ [31]. The B/G_H ratio of ErCu intermatallic compound is 2.50. This is clearly confirms that ErCu possess good ductility in B_2 type cubic structure.

3.3 Thermal Properties

The temperature plays significance role to determine the electronic and optical properties of material. We have used a quasi-harmonic approximation to obtain thermal properties. In energy ΔF, internal energy ΔE, entropy S and at constant volume specific heat C_v from 0 K to 1000 K of Er, Cu and ErCu intermatallic compound in Fig. 3(a-d). which we listed the contribution to the vibrational Fig. 3(a-d) depict that, at lower temperature (K), entropy S , Specific heat C_v and internal energy ΔE values increase with temperature and converged to constant values with higher temperature (K). As shown in Fig. 3(b), vibrational energy ΔF decrease of as temperature increases up to 1000 K range. As seen, Er atom has higher vibrational energy compare to that the Cu atom and ErCu compound. Moreover, At the 110 K temperature, the vibrational energy of Cu atom and ErCu compound is same and at 140 K temperature, again, the Er atom and ErCu meet at same energy. While At 250 K temperature, the vibrational energy of Er and Cu atom are same that predict that the ErCu has a most convenient vibrational energy with respect to the Er and Cu vibrational energy. From Fig. 3(c), we can see that, the entropy of ErCu is ~ 18 $J \cdot K^{-1} \cdot mol^{-1}$ that concluded that, the ErCu compound is not harder compound, which concludes that ErCu compound has a very high ductility.

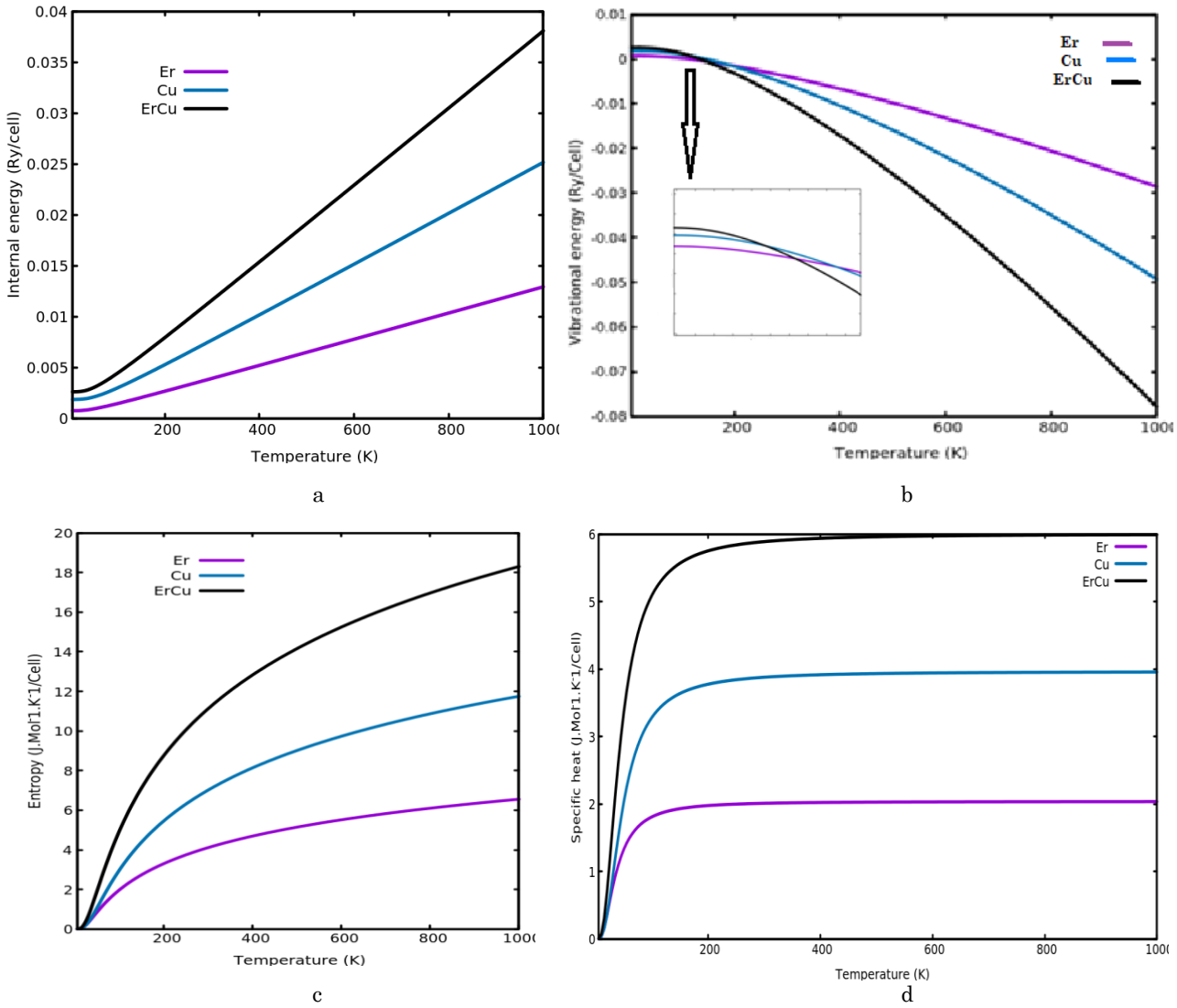

Fig. 3 – Internal energy variations with temperature for Er, Cu and ErCu (a); vibrational energy variations with temperature for Er, Cu and ErCu (b); entropy variation with temperature for Er, Cu and ErCu (c); at a constant volume, Specific heat variation with temperature for Er, Cu and ErCu

4. CONCLUSIONS

In summary, the phonon dispersion curves show the dynamical stability of the B_2 ErCu system. The phonon dispersive curves and phonon density of states are corresponding to each other. The overlapping of acoustic and optical modes brings the indication of the metallic nature of the ErCu. The entropy of ErCu is ~ 18 $J \cdot K^{-1} \cdot mol^{-1}$ that concluded that, ErCu compound is not quite considering as harder compound. The B/G_H ratio is 2.50, which also point out the excellent ductility of the ErCu compound in B_2 type cubic phase.

AKNOWLEDGEMENTS

The computer facility developed under DST-FIST level-I (No.SR/FST/PSI-097/2006 dated 20th December 2006 and No.SR/FST/PSI-198/2014 dated 21 November 2014) programmes of Department of Science and Technology, Government of India, New Delhi and support under DRS-SAP-I (No. F-530/10/DRS/2010 (SAP-I) dated November 2010 and No.F.530/17/DRS-II/2018 (SAP-I), dated 17 April 2018) of University Grants Commission, New Delhi are highly acknowledged. DR is thankful for the project fellowship under DRS-II-SAP (No.F.530/17/DRS-II/2018(SAP-I),dated 17/04/2018) of University Grants Commission, New Delhi.

REFERENCES

1. X. Tao, H. Chen, X. Li, Y. Ouyang, S. Liao, *Phys. Scr.* **83** No 4, 045301 (2011).
2. R.P. Singh, V.K. Singh, R.K. Singh, M. Rajagopalan, *Am. J. Condens. Matter. Phys.* **3** No 5, 123 (2013).
3. X. Tao, Y. Ouyang, H. Liu, F. Zeng, Y. Feng, Z. Jin, *Physica B: Condens. Matter* **399** No 1, 27 (2007).
4. M. Davis, J. Kuriplach, *Physica B: Condens. Matter*. **205**, 3 (1995).
5. J. Pierre, P. Morin, D. Schmitt, B. Hennion, *Journal de Physique* **39** No 7, 793 (1978).
6. Jian Liu, Th. George Woodcock, Nils Scheerbaum, Ol. Gutfleisch, *Acta Mater.* **57** No 16, 4911 (2009).
7. R.L. Fleischer, R.J. Zabala, *Metall. Trans. A* **21** No 10, 2709 (1990).
8. Y.J. Shi, Y.L. Du, G. Chen, G.L. Chen, *Mater. Trans.* **49** No 11, 2480 (2008).
9. S. Meenakshi, *Bull. Mater. Sci.* **37 No 6**, 1343 (2014).
10. M. Shugani, S.S. Chouhan, M. Aynyas, S.P. Sanyal, *Adv. Phys. Theor. Appl.* **19**, 83 (2013).
11. V. Srivastava, G. Pagare, S.P. Sanyal, M. Rajagopalan, *Phys. Stat. Sol.* **246** No 6, 1206 (2009).
12. E. Mamontov, H. O'Neill, Q. Zhang, W. Wang and D.J. Wesolowski, *J. Phys. Condens. Matter*. **24** No 7, 064104 (2012).
13. R. Sun, D.D. Johnson, *Phys. Rev. B* **87 No 10**, 104107 (2013).
14. I. Lukačević, S.K. Gupta, *J. Alloy. Compd.* **597**, 148 (2014).
15. V. Mankad, S.K. Gupta, I. Lukačević, P.K. Jha, *J. Phys. Conf. Ser.* **377**, 012076 (2012).
16. V.H. Mankad, S.K. Gupta, I. Lukačević, P.K. Jha, *Comp. Mater. Sci.* **65**, 536 (2012).
17. C. Davide, Erbium pseudo potential, https://sites.google.com/site/dceresoli/pse
18. J.P. Perdew, A. Zunger, *Phys. Rev. B* **23**, 5048 (1981).
19. N.E. Zein, *Sov. Phys. Solid State* **26**, 3028 (1984).
20. D.K. Blat, N.E. Zein, V.I. Zinenko, *J. Physics: Condens. Matter* **3** No 29, 5515 (1991).
21. N.E. Zein, *Phys. Lett. A* **161** No 6, 526 (1992).
22. S.S. Baroni, P. Giannozzi, A. Testa, *Phys. Rev. Lett.* **58**, 1861 (1987).
23. P. Giannozzi, S. de Gironcoli, P. Pavone, S. Baroni, *Phys. Rev. B* **43**, 7231 (1991).
24. S. Baroni, S. de Gironcoli, A. Dal Corso, P. Giannozzi, *Rev. Mod. Phys.* **73**, 515 (2001).
25. H.J. Monkhorst, J.D. Pack, *Phys. Rev. B* **13** No 12, 5188 (1976).
26. P. Giannozzi, *J. Phys. Condens. Matter*. **29**, 465901 (2017).
27. http://qeforge.qe- forge.org/gf/project/thermo_pw
28. D. Raval, B. Babariya, S.K. Gupta, P.N. Gajjar, *Physica B: Condens. Matter*. **570**, 122 (2019).
29. W. Setyawan, S. Curtarolo, *Comp. Mater. Sci.* **49** No 2, 299-312 (2010).
30. M. Born, K. Huang, *Am. J. Phys.* **23**, 474 (1995).
31. S.F. Pugh, *J. Sci.* **45** No 367, 823 (1954)