A benchmark for some bulk properties of bcc iron

E. Güler[1]* and M. Güler[1]
[1]Hitit University, Department of Physics,
19030 Corum-TURKEY

ABSTRACT

Some bulk properties of bcc iron were calculated. Structural and elastic properties such as cohesive energy, bulk modulus, typical elastic constants and vacancy formation energy were calculated for zero Kelvin temperature. All obtained results during the study were compared with the both previous experimental and theoretical results. Obtained results for the present study show well agreement with literature.

Keywords: bcc, EAM, bulk properties, LAMMPS, iron

1. INTRODUCTION

Calculations of the bulk structure and the bulk elastic properties play an important role in the physics of condensed matter [1-6]. Bulk calculations help us to understand, characterize, and predict mechanical properties of materials in our surroundings, under extreme conditions, as in geological formations and setting and for industrial applications [6-8]. Crystalline materials come in many different structures and in contrast to isotropic materials, the structure description of crystalline materials may in general need multiple lattice parameters and an atomic basis.

In this study we discuss how to determine the equilibrium structure of a crystalline material while, at the same time, directly determining the bulk modulus (B), cohesive energy (E_{coh}), vacany formation energy (E_V^F) and estimating other related physical parameters such as three independent cubic elastic constants (C_{11}, C_{12} and C_{44}) [9-11].

A theory determination of the zero-temperature bulk modulus based on either traditional methods is straightforward when one single structural parameter (e.g., the lattice parameter a_0) defines the crystalline state. This situation applies for monatomic crystals with simple cubic (sc), face-centered cubic (fcc) and body-centered cubic (bcc) symmetries. All which is required are theory calculations of total energies for a range of a_0 values by minimizing the energy of the related structures [1, 9].

Furthermore, atomic-scale simulations are nowadays a standard tool in condensed matter physics, chemistry and materials science. They enable a detailed investigation of material processes and phenomena with atomic resolution. One of the most efficient atomistic technique is free energy minimization method with the help molecular dynamics (MD) codes using interatomic potentials. The main goal of these potentials deals with determining reasonable results which are consistent with the experimental data [12].

According to simple metals persperctive, bcc iron and its alloys have been extremely used by many generations since the Iron Age. Their most useful property is high strength over a

---

*Corresponding author. E-mail: eguler71@gmail.com Tel:903642277000 Fax: 90364277005 wide range of application temperature and low cost, which makes them the ideal candidates for both structural and high temperature applications. Indeed, bcc iron alloys are and the most important structure material because of the abundance of iron ores on earth [13].

The purpose of this study was to clarify some aforementioned bulk physical parameters of bcc iron by free energy minization by the help of LAMMPS MD code and compare our present results with the previous experimental and theoretical data obtained from the various interatomic potentials.

2. METHODS AND CALCULATIONS

2.1. ENERGY MINIMIZATION AND BULK MODULUS

During the present study all energy minimizations have been perfomed by LAMMPS [14–15] code, with Finnis-Sinclair embedded atom potential [16]. For a bcc lattice and a given equation of state (EOS), E as a function of lattice parameter a_0 or volume $v = \square\frac{1}{2}a_0^3$, the bulk modulus B is defined by the equation

$$B = V\left(\frac{\partial^2 E}{\partial V^2}\right) = \frac{2a_0}{9}\left(\frac{\partial^2 E}{\partial a_0^2}\right)$$

evaluated at the minimum.

The position of the minimum of EOS defines the equilibrium lattice parameter and unit cell volume at zero pressure. The cohesive energy is then the difference between the energy per atom of the bulk material at equilibrium and the energy of a free atom in its ground state. To avoid interaction between an atom with its own periodic images, we consider a cubic simulation cell whose size is much larger than the cut-off radius. The cell dimensions are 10[100], 10[010] and 10[001] along x, y and z directions with a supercell containing $N = 2000$ atoms (because each unit cell of a bcc crystal contains 2 atoms). Periodic boundary conditions (PBC) are applied in all three directions. The experimental value of the equilibrium lattice constant (a_0) for Fe is = 2.87 Å. Therefore, to compute the equilibrium lattice constant of this potential model, we vary the lattice constant (a_0) from 2.6 Å to 3.1 Å, in steps of 0.1 Å. The potential energy per atom E as a function of a_0 is plotted in Fig. 1. According to literature [12,17] this data can be fitted to a parabola. Thus, we fitted this data to a third order polynomial.

2.2. ELASTIC CONSTANTS

The procedure to calculate elastic constants were directly applied as in Lammps manual which can be provided within the Lammps web site in Ref [14,15]. By using the definitions and comments from the Lammps software package we have calculated the elastic constants of Fe at zero Kelvin which this temperature directly stands for the ground state properties of the related element.

2.3. VACANCY FORMATION ENERGY

A vacancy is created when an atom within a perfect lattice is removed [18-19]. So, we firstly constructed a bcc perfect lattice with 2000 atoms at zero K. However, when an atom is removed from a crystal, the surrounding atoms will readjust their atomic positions to lower the potential energy. To obtain such a relaxed vacancy configuration one may use energy minimization techniques. Secondly, we removed one atom from the perfect crystal by using

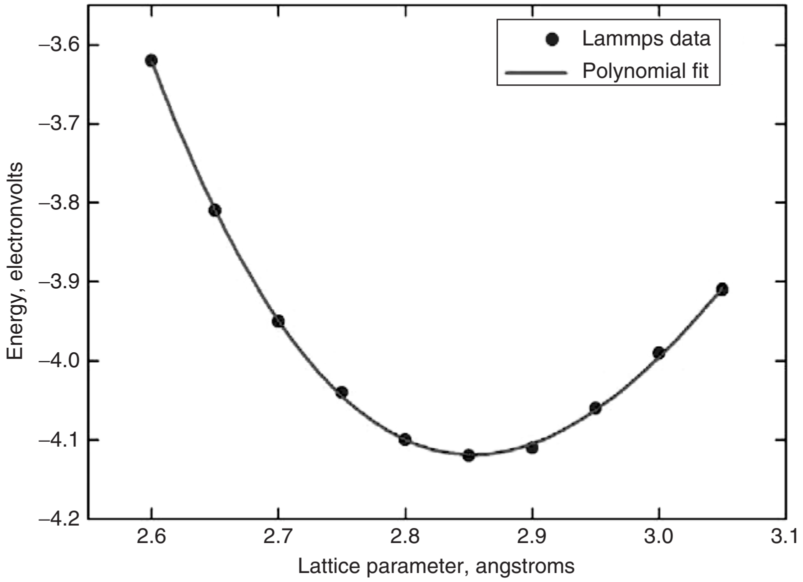

Figure 1 Lattice parameter versus energy.

conjugate gradient (CG) algorithm [20] for energy minimization with a NVT enseble [21]. For determination of the E_V^F we used the following relation [22]:

$$E_V^F = E_2 - \frac{N-1}{N} E_1$$

where E_1 is the perfect crystal energy with N atoms and E_2 is the relaxed energy of the system containing the vacancy with $N-1$ atoms.

3. RESULTS AND DISCUSSION

Figure 1 shows the energy change w.r.t lattice paramater for iron obtained from LAMMPS. The energy per atom at a_0 is the cohesive energy is found to be as $E_{coh} = -4.12$ eV. The curvature of parabolic curve at a_0 gives an estimate of the bulk modulus, $B = 178$ GPa. When comparing with the experimental values, the cohesive energy result shows a good agreement with the earlier literature values. Futhermore, the bulk modulus *(B),* which is an important parameter to characterize the mechanical behaviour of a material generally exhibits a good consistency with former results. As a defect formation energy in bcc iron, the vacancy formation energy (E_V^F), is found to be as 1.6 eV which this value also appears in the experimental range. On the other hand, Figure 2 indicates the change of elatics constants w.r.t. varying lattice constants of bcc iron. As it is obvious from Figure 2. C_{11} exhibits a linear increase where bulk modulus, C_{12} and C_{44} display a linear decrease with the increasing lattice parameter.

According to mechanical (dynamical) stability: $C_{11}–C_{12} > 0$, $C_{11} > 0$, $C_{11} + 2C_{12} > 0$ and cubic stability conditions i.e $C_{12} < B < C_{11}$ must be satisfied [23-24].

Finally, Figure 3 represents the comparison of present and prior findings on the cubic elatic constants of bcc iron through various interatomic potentials. It is clear from Fig. 3 that the results of Müller atomic bond order potential [9] provides much better values closer to

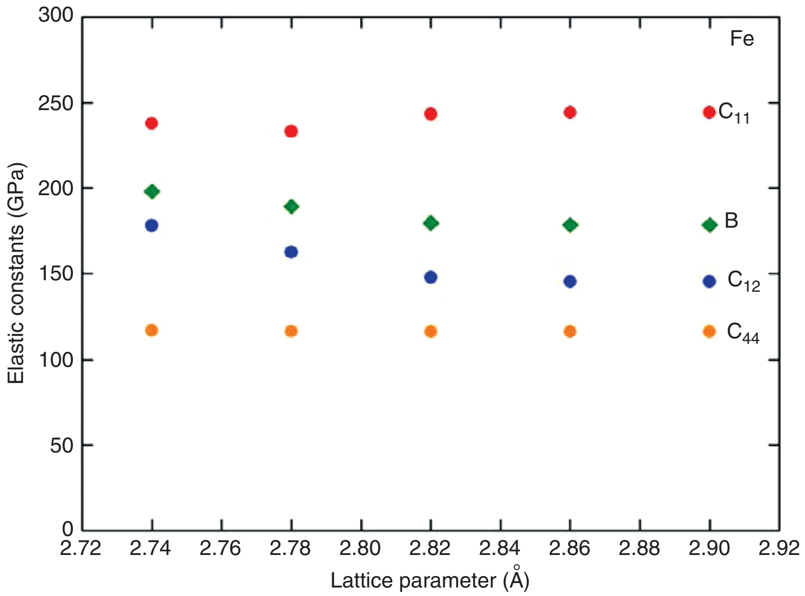

Figure 2 Change of elastic constants versus lattice parameter.

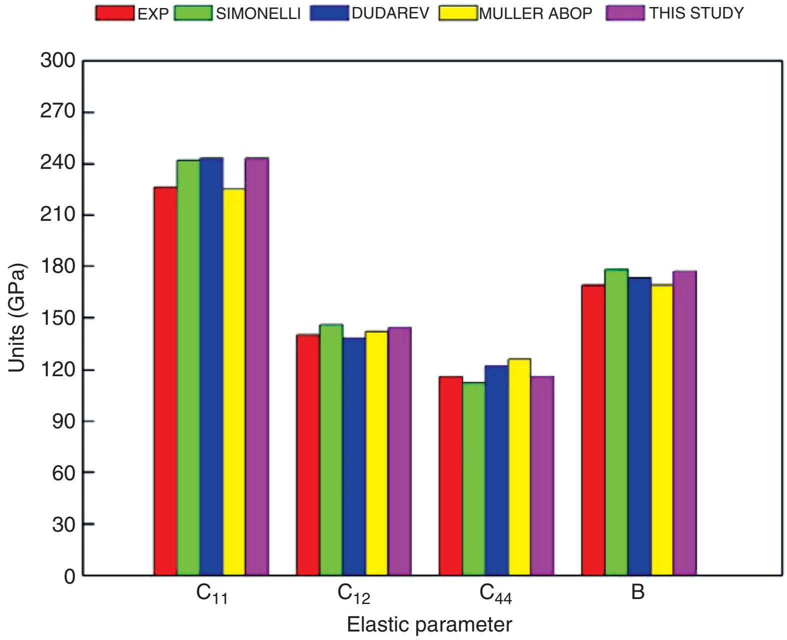

Figure 3 Comparison of present and previous results.

experimental findings. Additionally application of FS potential in the present study shows a similar result range with Simonelli et al results [26] and Dudarev and Derlet results [27]. All calculated parameters from molecular dynamics during the present study were given in Table 1.

Table 1 Some calculated and experimental physical parameters of bcc iron.

Parameter	**Exp**	**Simonelli[(a)]**	**Dudarev[(b)]**	**Müller[(c)] ABOP**	**This Study**
a_0 (Å)	2.87[(c)]	2.86	2.86	2.86	2.86
E_c (eV)	4.28[(c)]	4.28	4.12	4.28	4.12
E_V^F (eV)	1.5-1.8[(c)]	1.6	1.8	1.5	1.6
C_{11} (GPa)	226[(c)]	242	243	225	244
C_{12} (GPa)	140[(c)]	146	138	142	145
C_{44} (GPa)	116[(c)]	112	122	126	116
B (GPa)	169[(c)]	178	173	169	178

[(a)]Ref.26, [(b)]Ref.27, [(c)]Ref.28.

Also a considerable comparison can be seen with the former available experimental and previous theoretecal literature data for various interatomic potentials can be seen in Table 1.

4. CONCLUSION

We performed calculations to study the some structural and elastic properties of bcc iron for zero K temperature. The following conclusions have been drawn from present study:

- Bcc iron elastic constants are in good agreement with the prior available experimental and theoretically calculated literature values.
- Calculated elastic constants obey the structural stability conditions ($C_{11}–C_{12} > 0$, $C_{11} > 0$, $C_{44} > 0$,$C_{11} + 2C_{12} > 0$) which gives credence to our calculated values.
- Experimentally it is expensive and diffucult to obtain vacancy properties. Beacuse measurement of these experiments requires very pure samples and small concentrations of thermal vacancies for reliable results [25]. Therefore, with the appropriate interatomic potential present type of calculations provide good reults for vacancy defect calculations.

REFERENCES

[1] A. B. Alchagirov et al., Energy and pressure versus volume: Equations of state motivated by the stabilized jellium model, *Phys. Rev. B* , (2001), 63, p. 4115.

[2] P. Käckell, B. Wenzien, and F. Bechstedt**,** Influence of atomic relaxations on the structural properties of SiC polytypes from ab initio calculations, *Phys. Rev. B*, (1994), 50, p. 17037.

[3] C. Persson and E. Janzén, *J. Phys.: Condens. Matter*, Electronic band structure in hexagonal close-packed Si polytypes, 1998, 10, p. 10549.

[4] E. Schröder, Nematic liquid-crystal director configuration for general elastic coefficients, *Phys. Rev. E*, 2000, 62, p. 8830.

[5] E. Wachowicz and A. Kiejna, Bulk and surface properties of hexagonal-close packed Be and Mg, *J. Phys.: Condens. Matter.*, 2001, 13, p. 10767.

[6] Y. Yourdshahyan et al., First-principles calculations on the atomic and electronic structure of κ-Al_2O_3, *Phys. Rev. B*, 1997, 56, p. 8553.

[7] Y. Yourdshahyan et al., Theoretical Structure Determination of a Complex Material: κ-Al_2O_3, *J.Am. Ceram. Soc.*, 1999, 82, p. 1365.

[8] Y. Mishin et al., Interatomic potentials for monoatomic metals from experimental data and ab initio calculations, *Phys. Rev. B*, 1999, 59, p. 3393.

[9] M. Müler, P. Erhart and K. Albe, Analytic bond-order potential for bcc and fcc iron- comparison with established embedded-atom method potentials, *J.Phys.: Condens. Matter*. 2007, 19, 326220.

[10] F. D. Murnaghan, *Proc. Natl. Acad. Sci*., The Compressibility of Media under Extreme Pressures, 1944, 30, p. 244.

[11] F. Birch, Finite strain isotherm and velocities for single-crystal and polycrystalline NaCl at high pressures and 300°K, *J. Geophys. Res*., 1978, 83, p. 1257.

[12] V. V. Bulatov and Wei Cai, *Computer simulations of Dislocations*, Oxford University Press, 2006.

[13] D. Hull and D. J. Bacon: *Introduction to Dislocations*, 4th ed.,Butterworth Heinemann, Oxford, pp. 14–20 and pp. 110–114, 2001.

[14] S. Plimpton, Fast Parallel Algorithms for Short-Range Molecular Dynamics, *J. Comput. Phys*. ,1995, 117, p. 1.

[15] http://lammps.sandia.gov

[16] M. W. Finnis and J. E. Sinclair, A simple empirical N-body potential for transition metals**,** *Phil. MagA*. ,1984, 50, p. 45.

[17] F.D. Murnaghan, The Compressibility of Media under Extreme Pressures, *Proc. Natl. Acad. Sci*., 1944, 50, p. 244.

[18] L. Ventelon et al., Ab initio investigation of radiation defects in tungsten: Structure of self-interstitials and specificity of di-vacancies compared to other bcc transition metals, *J. Nuc. Mater.*, 2012, 425, p. 16.

[19] W.G. Wolfer, Fundamental Properties of Defects in Metals, *Compreh. Nuc. Mater.*, 2012, 1, 1.

[20] J. Uppenbrink, R. L. Johnston, J. N. Murrell, Modelling transition metal surfaces with empirical potentials, *Surface Sci*., 1994, 304, p. 223.

[21] K. Yin, D. Zou, J. Zhong, D. Xu, *Comput. Mater. Sci*., A new method for calculation of elastic properties of anisotropic material by constant pressure molecular dynamics, 2007, 38, p. 538.

[22] See Ref. 12.

[23] M. Wen, A. Barnoush, K. Yokogawa, Calculation of all cubic single-crystal elastic constants from single atomistic simulation: Hydrogen effect and elastic constants of nickel. *Comp. Phys. Comm*., 2011, 182, p. 1621.

[24] M. K. Niranjan, First Principles Study of Electronic, Optical and Elastic Properties of cubic anand Orthorhombic RhSi, *Intermetallics*, 2012, 26, p. 150.

[25] T. Korhonen, M. J. Puska and R. M. Nieminen, Vacancy-formation energies for fcc and bcc transition metals, *Phys. Rev. B*, 1995, 51, p. 9526.

[26] G.Simonelli, R. Pasianot, E. J. Savino, Embedded - Atom - Method Interatomic Potentials for BCC – Iron**,** *Mater. Res. Soc. Symp. Proc*., (1993) 291, p. 567.

[27] S. L. Dudarev and P.M. Derlet, A magnetic interatomic potential for molecular dynamics simulations, *J. Phys.: Condens. Matter*., 2005, 17, p. 7097.

[28] See Ref. 9