A benchmark for some bulk properties of bcc iron

E. Güler* and M. Güler

1Hitit 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 ($E_{coh}$), vacancy formation energy ($E^V$) 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 perspective, 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
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 performed 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 \( v = \frac{1}{2} a_0^3 \), 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
conjugate gradient (CG) algorithm [20] for energy minimization with a NVT ensemble [21]. For determination of the $E^F_V$ we used the following relation [22]:

$$E^F_V = E_2 - \frac{N-1}{N} E_1$$

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 ($E^F_V$), 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 elatics 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
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.

Figure 2 Change of elastic constants versus lattice parameter.

Figure 3 Comparison of present and previous results.
Also a considerable comparison can be seen with the former available experimental and previous theoretical 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 \( C_{11} - C_{12} > 0, \quad C_{11} > 0, \quad C_{44} > 0, \quad C_{11} + 2C_{12} > 0 \) which gives credence to our calculated values.
• Experimentally it is expensive and difficult to obtain vacancy properties. Because 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 results for vacancy defect calculations.

REFERENCES


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

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Exp</th>
<th>Simonelli(^{(a)})</th>
<th>Dudarev(^{(b)})</th>
<th>Müller(^{(c)})</th>
<th>ABOP Study</th>
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<tbody>
<tr>
<td>(a_0) (Å)</td>
<td>2.87(^{(c)})</td>
<td>2.86</td>
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<td>(E_c) (eV)</td>
<td>4.28(^{(c)})</td>
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<td>(E_V) (eV)</td>
<td>1.5-1.8(^{(c)})</td>
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<td>1.8</td>
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<td>1.6</td>
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<td>(C_{11}) (GPa)</td>
<td>226(^{(c)})</td>
<td>242</td>
<td>243</td>
<td>225</td>
<td>244</td>
</tr>
<tr>
<td>(C_{12}) (GPa)</td>
<td>140(^{(c)})</td>
<td>146</td>
<td>138</td>
<td>142</td>
<td>145</td>
</tr>
<tr>
<td>(C_{44}) (GPa)</td>
<td>116(^{(c)})</td>
<td>112</td>
<td>122</td>
<td>126</td>
<td>116</td>
</tr>
<tr>
<td>(B) (GPa)</td>
<td>169(^{(c)})</td>
<td>178</td>
<td>173</td>
<td>169</td>
<td>178</td>
</tr>
</tbody>
</table>

\(^{(a)}\)Ref.26, \(^{(b)}\)Ref.27, \(^{(c)}\)Ref.28.
[22] See Ref. 12.
[28] See Ref. 9