Structural, elastic and thermal properties of Laves phase Fe$_2$Mo from first principles

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Abstract. In this work, structural, elastic and thermal properties of the Laves phase Fe$_2$Mo ($\lambda$-) with the C14-type structure existing in the Fe – Mo system have been investigated using the quantum mechanical calculations within the frame of the density functional theory (DFT). The equilibrium lattice parameters, atoms position coordinates and average magnetic moment of atoms were calculated. The five independent elastic constants of the strain tensor were calculated by imposing small strains on the crystal lattice. Polycrystalline elastic parameters: bulk modulus ($B$), shear modulus ($G$), Young’s modulus ($E$), and Poisson’s ratio ($\nu$) were obtained by using the Voigt-Reuss-Hill (VRH) approximation. An assessment of anisotropy of elastic properties was carried out. The Debye temperature and anisotropic sound velocities were predicted. The calculated results were analyzed. The obtained results are useful to improve the understanding of the physical and chemical nature of the Fe$_2$Mo phase.

1. Introduction

Ferritic steels are both fundamental and industrial interest, and considered as promising for use as fuel element cladding of the new generation reactors IV, as well as the first wall of future fusion reactors. This is due to their low creep, good corrosion resistance and low swelling at elevated temperatures [1, 2]. Long duration of the material exploitation under irradiation and elevated temperatures is responsible for kinetic processes, due to diffusion, which lead to the changes of its structural and physical properties that in turn can lead to cracking and fracture of the material.

The Fe-Mo system is a base for development of ferritic steels, it possesses the Laves phase Fe$_2$Mo ($\lambda$-), µ-, R-, σ- and γ-phases. These phases essentially limit the stable area of bcc solid solutions. Knowledge of the location of these phase boundaries on the Fe-Mo phase diagram is necessary for the successful design of materials used in industry. In construction steels, the Laves phase is a hardening phase, which precipitated during heating or operation of a product for a long time at high temperature. A characteristic feature of the Laves phase is their slow precipitation from solid solution and the slow growth of particle sizes, which favourably affects the stabilization of the mechanical properties that occur during long isothermal exposures [3]. Knowledge of the thermodynamic properties for the Fe$_2$Mo phase is important not only for constructing phase diagrams of binary and ternary (for example, Fe-Cr-Mo) systems, as well as for understanding the kinetic processes taking place in these materials. The experimental obtaining of thermodynamic properties depending on the temperature of the phase presents...
significant difficulties. These difficulties are connected with the fact that this phase is in the low-
temperature part of the phase diagram where diffusion processes are slow, as well as the presence of
other phases, such as $\mu$-, $R$- and $\sigma$-. For understanding the diffusion processes taking place in these
materials is expedient to conduct the computer simulations and obtain Gibbs potentials.

The use of quantum mechanical calculations is important for calculating the energy (and enthalpy)
of the formation of the Fe$_2$Mo in the ground state (at $T = 0$ K), as well as for obtaining the temperature
dependence of the Gibbs potential. To calculate them, it is necessary to calculate the equilibrium
parameters of the crystal lattice, the elastic constants ($C_{ij}$) of the strain tensor, and the Debye temperature
of the Laves phase Fe$_2$Mo.

Several studies on the structural properties and lattice stabilities of Fe$_2$Mo have been conducted over
the past years. Rajkumar et al. [5] reported the lattice parameters, the formation enthalpy and
thermodynamic functions of Fe-Mo alloys, using CALPHAD approach and Density Functional Theory
(DFT). Lejeaghere et al. [6] obtained lattice parameters, optimized atoms positions of Fe$_2$Mo and total
magnetic moments with the help of the DFT calculations. Pavlu et al. [7] predicted the lattice parameters
and Bulk modulus of Fe$_2$Mo by DFT. From above, one could see that these studies are mainly focusing
on structure properties of Fe$_2$Mo. However, despite a great importance of developing the ferrite steels,
the elastic and thermal properties of Fe$_2$Mo are not well compared and reported at the same time. Since
these data are important for constructing Gibbs energy and calculating the physical and chemical
properties of Fe-Mo alloys, their absence was a motivation prompted to study them.

In this paper, first principles theoretical calculations were carried out to investigate the structure,
elastic and thermal properties of the Fe$_2$Mo compound. The structure was optimized by full relaxation
and the lattice parameters were obtained. The heat of formation energy was calculated. The elastic
constants, $C_{ij}$, were obtained by implying small strains on the lattice and calculating the corresponding
total energies. Then, the bulk modulus $B$ and shear modulus $G$, Young’s modulus $E$, and Poisson’s ratio
$\nu$ were obtained by using the Voigt-Reuss-Hill (VRH) approximation. After, the Debye temperature,
sound velocities in different directions and anisotropy parameters were derived. The ductility, plasticity
and other mechanical properties of this compound were discussed. The presented results were obtained
from first principles, which mean that only atomic numbers of elements were used as input parameters.
The results give a valuable estimation for the properties which very difficult to obtain in experiments.

2. Computational methods
The calculations were performed by the first principles calculations implemented in the WIEN2k
package [8], which employs the Full Potential-Linear Augmented Plane Wave (FP-LAPW) Method [8]
based on the density functional theory (DFT) [9, 10]. The exchange and correlation terms were described
by the generalized gradient approximation (GGA) with the Perdew-Bruke-Eruzerhof (PBE) functional
[11]. The parameters $RK_{\text{max}}$ (the minimum radius times the maximum plane-wave coefficient) and
muffin-tin radius ($R_{\text{MT}}$) were set as $R_{\text{MT}} = 2.05$ for Fe, $R_{\text{MT}} = 2.15$ for Mo and $RK_{\text{max}} = 9$. To model the
Fe$_2$Mo compound the cell of 12 atoms was used with a 13 x 13 x 6 $k$-point mesh in the first irreducible
Brillouin zone using Monkhorst-Pack scheme [12]. To confirm the convergence of the calculations, a
careful investigation of the dependence of the total energy on the size of the grid for the $k$-point mesh
was carried out. The structure optimizations were performed by full relaxation until the maximum force
on the atom was below 0.005 eV/Å and the maximum stress was below 0.02 GPa. The calculations of
total energy and electronic structure are followed by cell optimization with self-consistent field (SCF)
tolerance of 5x$10^{-6}$ eV/atom.

3. Results and discussion
3.1. Crystal structure and lattice constants
The Fe₂Mo phase is a stoichiometric compound with the fixed composition and possess the hexagonal MgZn₂ structure, with space group \(P6_3/mmc\) (No. 194) and Pearson symbol is hP12, as shown in figure 1. It contains 8 Fe atoms and 4 Mo atoms in the unit cell, where the Fe atoms occupy the 2a Wyckoff site (0, 0, 0) and 6h site (0.830, 0.660, 0.250), Mo atoms occupy the 4f site (0.333, 0.667, 0.063).

In order to investigate the ground-state properties of Fe₂Mo, the spin-polarized calculations with the geometry optimizations and the full structural relaxation optimization have been performed from the above configuration. The optimized lattice parameters are listed in table 1, together with the available experimental values [7, 13, 14] and other theoretical results [5, 6, 7, 15, 16] for comparison. Note that the obtained equilibrium lattice parameters are all in agreement with the experimental results within 1.5%, suggesting that the calculations in the present work are reasonable. The calculated enthalpy formation of the Fe₂Mo phase is negative meanings that the compound is stable, the obtained value is shown in table 1 together with the other theoretical values. The obtained optimized atomic coordinates are given in table 2. Their comparison with the theoretical results [6] is showing a satisfactory agreement within 1 %. Spin magnetic moments are reported as well in table 2. Details about the enthalpy formation calculations of Fe₂Mo see the next section.

### Table 1. Calculated lattice constants (in Å), equilibrium volume \(V\) (in Å³), formation enthalpies \(\Delta H\) (kJ/mol) of Laves phase Fe₂Mo, together with available experimental and other theoretical values.

| Phase  | Method | \(a\)  | \(c\)  | \(c/a\) | \(V\)  | \(\Delta H\) |
|--------|--------|--------|--------|--------|--------|------------|
| Fe₂Mo  | This work | 4.672  | 7.775  | 1.664  | 147.004 | -2.210     |
|        | Exp. [14] | 4.73   | 7.72   | 1.632  | 149.579 |            |
|        | Exp. [7]  | 4.745  | 7.734  | 1.630  | 150.802 |            |
|        | Exp. [13] | 4.731  | 7.768  | 1.642  | 150.573 |            |
|        | Calc. [7] | 4.682  | 7.560  | 1.615  | 145.531 |            |
|        | Calc. [6] | 4.659  | 7.743  | 1.662  | 145.585 |            |
|        | Asses. [16] | 4.744 | 7.725  | 1.628  | 150.563 |            |
|        | Calc. [5] | 4.669  | 7.793  | 1.669  | 147.124 | -0.714     |
|        | Calc. [15] | -      | -      | -      | 147.124 | -1.534     |

* Obtained at \(T = 1073\) K after 1500 hours of annealing.

### Table 2. Calculated atomic coordinates of Fe₂Mo. Spin magnetic moments per atom are given within spheres with radius \(R_{MT}\). The total magnetic moment in cell (including the interstitial space) is 4.451 (\(\mu_B\)) for Laves phase Fe₂Mo.

| Element | Site | \(x\)     | \(y\)     | \(z\)     | Moment (\(\mu_B\)) |
|---------|------|-----------|-----------|-----------|---------------------|
| Fe      | 2a   | 0.00000   | 0.00000   | 0.00000   | -1.241              |
| Fe      | 6h   | 0.17050   | 0.34100   | 0.75000   | +1.195              |
| Mo      | 4f   | 0.33333   | 0.66667   | 0.06978   | -0.034              |
3.2. Heat of formation

In order to have a measure about the relative phase stability of Fe$_2$Mo the formation enthalpy ($\Delta H$) was calculated by performing spin-polarized calculations. Negative formation enthalpy means an exothermic process, and the lower energy indicates the stability with respect to the decomposition to elemental constituents. The formation enthalpy of Fe$_2$Mo can be calculated by the following expression [17]:

$$\Delta H^{AB} = E_{\text{total}}^{AB} - (x E_{\text{solid}}^A + (1-x) E_{\text{solid}}^B)$$

where $E_{\text{total}}^{AB}$ is the total energy of the unit cell of the considered compound, $E_{\text{solid}}^A$ and $E_{\text{solid}}^B$ denote the energies of Fe and Mo atoms in the solid state (i.e. in the body centred cubic (bcc) lattice), respectively; $x$ is the concentration of Mo atoms ($x = 0.333$). The calculated formation enthalpy of Fe$_2$Mo is reported in table 1 together with the other theoretical values obtained by different authors. It is shown that the formation enthalpies of Fe$_2$Mo compound is negative, implying that the phase is stable from the energetic point of view.

3.3. Elastic properties

The elastic constants, $C_{ij}$, determine the response of the crystal to extra forces, as characterized by bulk modulus $B$, shear modulus $G$, Young’s modulus $E$, and Poisson’s ratio $\nu$. So $C_{ij}$ play an important part in the mechanical properties of material science.

To calculate the elastic constants $C_{ij}$, external small stress needed to be applied to the equilibrium lattice and the corresponding variation in the total energy needed to be determined. The elastic strain energy was given as follows [18]:

$$U = \frac{\Delta E}{V_0} = \frac{1}{2} \sum_i \sum_j C_{ij} e_i e_j$$

where $\Delta E = E_{\text{total}}(V, \delta) - E_{\text{total}}(V_0, 0)$ is the total energy difference between deformed cell and the initial cell, $V_0$ is the volume of equilibrium cell and $C_{ij}$ are the elastic constants; $e_i$ and $e_j$ are strains, $\delta$ is the deformation added to the equilibrium cell. The elastic constants are identified as proportional to the second order coefficient in a polynomial fit of the total energy as a function of the distortion parameter $\delta$ [18].

The Fe$_2$Mo phase can be described by a hexagonal crystal lattice which has two parameters $a$ and $c$ with Bravais lattice vectors of matrix form:
\[ R = \begin{pmatrix} \frac{\sqrt{3}}{2}a & -\frac{1}{2}a & 0 \\ -\frac{1}{2}a & \frac{\sqrt{3}}{2}a & 0 \\ 0 & 0 & \frac{c}{a} \end{pmatrix} \]  

The linear combinations of elastic constants, \( C_{ij} \), were determined by straining the lattice vectors \( R \) according to the relation \( R' = RD \), where \( R' \) is the deformed matrix with distorted lattice vectors and \( D \) is the symmetric distortion matrix, which contains the strain components \( \delta \). Since, for a hexagonal structure, there are five independent elastic constants \( (C_{11}, C_{12}, C_{13}, C_{33}, C_{44}) \) and one dependent constant which is calculated as \( C_{66} = (C_{11} + C_{12})/2 \) [19], we need five different strains to determine them. The five distortion matrices, \( D_i \), used in the present calculations are given in Table 3 with the corresponding formulas of changes in the energy as a function of applied strain. The feature of the \( D_2, D_3 \) and \( D_5 \) matrices is when they are used to distort the lattice, the volume remains constant. The method utilizing these distortion matrices for calculating the elastic constants, \( C_{ij} \), have been described by Ravindran et al. [20].

**Table 3.** Distortion matrices for calculating the elastic constants for the Fe\(_2\)Mo compound. The constants \( C_{ij} \), were evaluated from the energy changes corresponding to applied strains.

| Distortion matrix | Energy change due to applied strain |
|-------------------|-----------------------------------|
| \( D_1 \) = \begin{pmatrix} 1 + \delta & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} | \[ \Delta E = V_0(\tau_1 \delta + \frac{C_{11}}{2} \delta^2) \] |
| \( D_2 \) = \begin{pmatrix} 1 + \delta & 0 & 0 \\ 0 & 1 - \delta & 0 \\ 0 & 0 & \frac{1}{(1 - \delta^2)^{1/3}} \end{pmatrix} | \[ \Delta E = V_0 \left[ (\tau_1 - \tau_2) \delta + \frac{1}{2} (C_{11} + C_{22} - 2C_{12}) \delta^2 \right] \] |
| \( D_3 \) = \begin{pmatrix} 1 + \delta & 0 & 0 \\ 0 & 1 - \delta & 0 \\ 0 & 0 & \frac{1}{(1 - \delta^2)^{1/3}} \end{pmatrix} | \[ \Delta E = V_0 \left[ (\tau_1 - \tau_3) \delta + \frac{1}{2} (C_{11} + C_{33} - 2C_{13}) \delta^2 \right] \] |
| \( D_4 \) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 + \delta \end{pmatrix} | \[ \Delta E = V_0 (\tau_3 \delta + \frac{C_{33}}{2} \delta^2) \] |
| \( D_5 \) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{(1 - \delta^2)^{1/3}} & \delta \\ 0 & \frac{\delta}{(1 - \delta^2)^{1/3}} & \frac{1}{(1 - \delta^2)^{1/3}} \end{pmatrix} | \[ \Delta E = V_0 (2\tau_4 \delta + 2C_{44} \delta^2) \] |
So, the five distortion matrices, $D_i$, were applied to deform the lattice of Fe$_2$Mo, and the relevant energy dependencies necessary to calculate the required elastic constants were obtained. For each kind of lattice deformation, the total energy has been calculated for different strains $\delta = \pm 0.01n$. The changes in total energy ($\Delta E$) versus strain $\delta$ for Fe$_2$Mo for the five different types of distortions which listed in table 3 are plotted in figure 2. The five values of the second order coefficients, which were corresponding to $C_{11}/2$, $(C_{11}+C_{22}-2C_{12})/2$, $(C_{11}+C_{33}-2C_{13})/2$, $C_{33}/2$ and $2C_{44}$, were extracted respectively. By resolving the corresponding linear equations, the five elastic constants were obtained. The calculated results of the elastic constants for Fe$_2$Mo compound are listed in table 4. However, as far as is known, in literature, there aren’t any available experimental or theoretical values of the elastic constants for Fe$_2$Mo.

**Figure 2.** Changes in the strain energy ($\Delta E = E_{\text{tot}}(V, \delta_i) - E_{\text{tot}}(V_0, 0)$, Ry/cell) as a function of strain ($\delta$) for Laves phase Fe$_2$Mo. The blue circles represent the calculated values and the dotted line is the polynomial fit.
The generalized mechanical stability criteria for hexagonal crystals at zero pressure apply the following restrictions on the elastic constants [19]:

\[ C_{11} > 0, \quad C_{11} - |C_{12}| > 0, \quad (C_{11} + C_{12})C_{33} - 2C_{13}^2 > 0, \quad C_{44} > 0 \]  

(4)

Table 4. The calculated elastic constants \( C_{ij} \) (in GPa) of single crystal of Laves phase Fe\(_2\)Mo.

| Compound | \( C_{11} \) | \( C_{12} \) | \( C_{13} \) | \( C_{33} \) | \( C_{44} \) | \( C_{66} \) |
|----------|--------------|--------------|--------------|--------------|--------------|--------------|
| Fe\(_2\)Mo | 459.27       | 170.38       | 105.49       | 379.00       | 113.73       | 144.44       |

As one could see in table 4, that the obtained elastic constants for Fe\(_2\)Mo satisfy that criteria and as follow this compound is mechanically stable at zero pressure. The values of elastic constants \( C_{11} \) and \( C_{33} \) reflect the stiffness against principal strains change, the value of \( C_{66} \) describes the resistance to shear in the \{100\} plane in the <110> direction, while \( C_{44} \) is a value of the resistance to shear in the \{010\} or \{100\} plane in the <001> direction. The large values of \( C_{11} \) and \( C_{33} \) for this compound can reflect a fact that its compression under the uniaxial stress along \( a \)-\( (\varepsilon_{11}) \) or \( c \)-\( (\varepsilon_{33}) \) axis may be hard.

However, in practice engineering, the polycrystalline elastic properties as bulk modulus \( B \), shear modulus \( G \), Young’s modulus \( E \) and Poisson’s ratio \( \nu \) are very valuable for determining the mechanical properties of materials. These polycrystalline elastic properties can be estimated directly from the single-crystal elastic constants, by using the Voigt-Reuss-Hill (VRH) approximation [21]:

\[
B = \frac{1}{2} (B_V + B_R), \quad G = \frac{1}{2} (G_V + G_R) 
\]

(5)

\[
E = \frac{9GB}{3B + G}, \quad \nu = \frac{3B - E}{6B} = \frac{E - 2G}{2G} 
\]

(6)

In formulas, the \( V \) and \( R \) indicate the model of Voigt and Reuss, respectively. The Voigt formulas provide the upper assessments of values of mechanical modulus while the Reuss formulas provide their lower assessments. The moduli of hexagonal crystals are described as follow [22]:

\[
B_V = \frac{1}{9} \left( 2(C_{11} + C_{12}) + 4C_{13} + C_{33} \right) 
\]

(7)

\[
B_R = \frac{(C_{11} + C_{12})(C_{33} - 2C_{13}^2)}{C_{11} + C_{12} + 2C_{33} - 4C_{13}} 
\]

(8)

\[
G_V = \frac{1}{30} \left( C_{11} + C_{12} + 2C_{33} - 4C_{13} + 12C_{44} + 12C_{66} \right) 
\]

(9)

\[
G_R = 15/(14S_{11} + 4S_{33} - 8S_{13} - 10S_{12} + 6S_{44}) 
\]

(10)

Where \( C_{ij} \) are elastic constants and \( S_{ij} \) are components of the compliances tensor, which is the inverse matrix of \( C_{ij} \). The obtained elastic compliances of single crystal of Laves phase Fe\(_2\)Mo are listed in table 5.

Table 5. Elastic compliances \( S_{ij} \) (in TPa\(^{-1}\)) of single crystal of Laves phase Fe\(_2\)Mo.

| Compound | \( S_{11} \) | \( S_{12} \) | \( S_{13} \) | \( S_{33} \) | \( S_{44} \) | \( S_{66} \) |
|----------|--------------|--------------|--------------|--------------|--------------|--------------|
| Fe\(_2\)Mo | 2.724        | -0.737       | -1.191       | 7.107        | 8.793        | 6.923        |

The moduli of polycrystalline aggregate of Fe\(_2\)Mo calculated by VRH approximation are listed in table 6. The bulk modulus \( B \) is a measure of resistance to volume change by applied pressure, and shear modulus \( G \) is a measure of resistance to reversible deformations upon shear stress [23].

Table 6. The calculated elastic modulus (in GPa) and Poisson’s ratio \( \nu \) of polycrystalline aggregate of Laves phase Fe\(_2\)Mo.

| Compound | \( B_V \) | \( B_R \) | \( B \) | \( G_V \) | \( G_R \) | \( G \) | \( E \) | \( \nu \) | \( B/G \) |
|----------|----------|----------|--------|----------|----------|--------|--------|--------|--------|
| Fe\(_2\)Mo | 228.9    | 224.1    | 226.5  | 135.5    | 110.1    | 122.8  | 312.0  | 0.27   | 1.84   |
In material science there is a concept of material plasticity it includes among other brittleness and ductility. In order to have an estimation of brittle or ductile behaviour of materials Pugh [23] have proposed the ratio of bulk modulus to shear modulus ($\frac{B}{G}$). A high value of $\frac{B}{G}$ ratio reflects the ductile behaviour of materials, whereas a low value associated with the brittle behaviour. The critical value which separate ductile and brittle material was suggested as 1.75. Levandovski et al. [24] proposed, that Poison’s ratio can represent such separation as well with the critical value of $\nu = 0.26$, so a material with $\nu > 0.26$ is referred to as having a ductile nature. Polycrystalline aggregate of Fe$_2$Mo was suggested to be ductile because it meets both these criteria, table 6.

Thus, calculated values of $\frac{B}{G}$ ratio and Poison’s ratio predict that Laves phase Fe$_2$Mo is a material with ductile behaviour. This ductile nature of Laves phase Fe$_2$Mo precipitating in a ferritic matrix of steel is one of the reasons why this phase is considered as a useful hardening phase.

### 3.4. Elastic anisotropy

In material science an ability to predict micro-cracks development in materials has an important application, and knowledge of elastic anisotropy of crystals during a material design is essential for preventing materials failure working under high load and high temperature [26]. Indications of the elastic anisotropy among other are the shear anisotropy factors ($A$), anisotropy in linear bulk modulus ($B_a$ and $B_c$), the percentage of anisotropy in the compression ($A_B$) and shear ($A_G$), the elastic anisotropy index ($A_U$) and the anisotropic elastic waves velocities.

The shear anisotropy factors: $A_{\{100\}}$ – between <011> and <010> directions for the {100} shear plane; and $A_{\{001\}}$ – between <110> and <010> directions for the {001} plane were given in the work [20].

$$A_{\{100\}} = \frac{4C_{44}}{C_{11} + 2C_{33} - 2C_{13}}$$

$$A_{\{001\}} = \frac{4C_{66}}{C_{11} + 2C_{22} - 2C_{12}}$$

The calculated results of $A_{\{100\}}$ and $A_{\{001\}}$ for Fe$_2$Mo are listed in table 7. The $A$ value of 1 (or 100%) indicates that a crystal is fully isotropic, while the value of 0 reflects its maximum anisotropy [23]. From these calculated values one can see that on {100} plane the Fe$_2$Mo has high anisotropy and isotropy on {001} plane.

The linear bulk modulus along the $a$- axis and $c$- axis were given by [20]

$$B_a = a \frac{dP}{da} = \frac{\Lambda}{2 + \beta}$$

$$B_c = c \frac{dP}{dc} = \frac{B_a}{\beta}$$

$$\Lambda = 2C_{11} + 2C_{12} + 4C_{13}\beta + C_{33}\beta^2$$

$$\frac{B_c}{B_a} = \frac{C_{33} - C_{13}}{C_{11} + C_{12} - 2C_{13}}$$

Where $\beta$ is defined as the relative change of the $c$-axis as a function of the deformation of the $a$-axis.

The value of $B_c/B_a$ ratio reflects the anisotropy of linear compressibility along the $c$-axis with respect to the $a$-axis. The calculated values of linear bulk modulus $B_a$ and $B_c$ listed in table 7 show the ratios of $B_c/B_a$ for Fe$_2$Mo, which indicate that the elastic anisotropy of that compound is in the middle range.

**Table 7.** The calculated shear anisotropic factors $A$ in the {100} and {001} directions, linear bulk modulus $B_a$ and $B_c$ (in GPa), and percentage of anisotropy $A_B$ and $A_G$ (in %) of Fe$_2$Mo.

| Compound | $A_{\{100\}}$ | $A_{\{001\}}$ | $B_a$  | $B_c$  | $A_B$  | $A_G$  | $B_c/B_a$ |
|----------|----------------|----------------|-------|-------|--------|--------|----------|
| Fe$_2$Mo | 0.725          | 1.000          | 791.13| 516.83| 1.070  | 10.322 | 0.653    |
The percentage of anisotropy in the compression $A_B$ and shear $A_G$ are another indication of anisotropy, and defined [20]

$$A_B = \frac{B_{UV} - B_R}{B_{UV} + B_R}$$  \hspace{1cm} (17)

$$A_G = \frac{G_{UV} - G_R}{G_{UV} + G_R}$$  \hspace{1cm} (18)

Where $B$ and $G$ are bulk and shear modulus, for these two expressions, a value of zero represents elastic isotropy and a value of 1 (or 100%) is the largest possible anisotropy. The calculated values of $A_B$ and $A_G$ are listed in table 7 show that Fe$_2$Mo is a material with isotropy elastic properties.

The elastic anisotropy index $A_U$ was proposed as a numerical index to represent the degree of elastic anisotropy of single crystal and is calculating as follow [25]

$$A_U = 5\frac{G}{G_R} + \frac{B}{B_R} - 6$$  \hspace{1cm} (19)

The calculated elastic anisotropy index of Fe$_2$Mo is 1.173.

About the anisotropic elastic waves velocities see the next section.

### 3.5 Thermal properties

The Debye temperature, $\theta_D$, is a fundamental parameter of thermodynamic, and is found in equations describing physical properties such as specific heat, thermal expansion, elastic constants, vibration entropy and melting temperature, which arise from theories involving atomic vibrations.

The value of the Debye temperature can be calculated from elastic constants since it proportional to the averaged sound velocity by the equation [27]

$$\theta_D = \frac{\hbar}{k_B} \left[ \frac{3n}{4\pi} \left( \frac{N_A \rho}{M} \right) \right]^{1/3} V_m$$  \hspace{1cm} (20)

Where $\hbar$ and $k_B$ are the Plank and the Boltzmann constants, $N_A$ is Avogadro constant, $\rho$ is the density, $n$ is the number of atoms per formula unit, $M$ is the molecular weight of the solid, $V_m$ is the average velocity of sound in polycrystalline material and can be calculated by

$$V_m = \left[ \frac{1}{3} \left( \frac{2}{V_s^2} + \frac{1}{V_l^2} \right) \right]^{-1/3}$$  \hspace{1cm} (21)

Where $v_s$ and $v_l$ are shear and longitudinal elastic wave velocities, respectively, which can be obtained using the polycrystalline bulk modulus $B$ and shear modulus $G$ from Navier’s equation as follows [27]

$$V_s = \left( \frac{G}{\rho} \right)^{1/2} \hspace{1cm} V_l = \left( \frac{(B + 4G/3)}{\rho} \right)^{1/2}$$  \hspace{1cm} (22)

The calculated results of elastic wave velocities ($v_s$, $v_l$, $V_{3h}$) and $\theta_D$ for Fe$_2$Mo are listed in table 8. The obtained density of Fe$_2$Mo compound is 9.38 (g/sm$^3$). According to the empirical rule, the higher the Debye temperature is, the better the thermal conductivity of the material. So, the predicted $\theta_D$ can be a measure of Fe$_2$Mo thermal conductivity. Another important feature of $\theta_D$ is the using in calculations of Gibbs potential depending on temperature in the frame of Debye- Grüneisen approach by taking anharmonic effects into account. As far as is known, there is no experimental or theoretical value of Debye temperature and sound velocities available for the Fe$_2$Mo phase. Thus, these results are of academic interest and may be usable for future works.

**Table 8.** The calculated average ($V_m$), shear ($v_s$) and longitudinal ($v_l$) elastic wave velocities (in m/s); predicted Debye temperature $\theta_D$ (in K), and elastic wave velocities along [001] and [100] directions (in m/s) of Laves phase Fe$_2$Mo.
The single-crystal elastic wave velocities in different directions can be obtained from the calculated elastic constants by solving the Cristoffel equation [28]:

$$[c_{ijkl}n_in_i - \rho V^2 \delta_{ik}] = 0$$

(23)

where $c_{ijkl}$ is the single-crystal elastic constant tensor, $n$ is the propagation direction, $\rho$ is the density, $V$ is the elastic wave velocity, and $\delta_{ik}$ is the Kroenecker delta function. There are two types of solutions of this equation: 1) sound velocity of a longitudinal wave $V_L$ and 2) two sound velocities of shear waves $V_{S1}$ and $V_{S2}$. For hexagonal crystal, the velocities of elastic waves propagating along [001] direction defined as following [29]:

$$V_L = \left(\frac{c_{33}}{\rho}\right)^{1/2}, \quad V_{S1} = V_{S2} = \left(\frac{c_{44}}{\rho}\right)^{1/2}$$

(24)

And the velocities of elastic waves propagating along [100] direction are given as:

$$V_L = \left(\frac{c_{11}}{\rho}\right)^{1/2}, \quad V_{S1} = \left(\frac{c_{66}}{\rho}\right)^{1/2}, \quad V_{S2} = \left(\frac{c_{44}}{\rho}\right)^{1/2}$$

(25)

The calculated results of anisotropic elastic waves velocities are shown in table 8. The fastest propagation of elastic waves was found along the [100] direction by longitudinal waves. Prediction of elastic wave velocities in different directions of the crystal can be useful for experimental studies.

4. Conclusions

In summary, the first-principles calculations were carried out to study the structural, elastic and thermal properties of the Laves phases Fe$_2$Mo. The calculated equilibrium lattice parameters, atoms position coordinates and its average magnetic moments for this compound are in a good agreement with available experimental and other theoretical values. The calculated formation enthalpy is negative and showing its structural stability. The strain energies for five different distortions of Fe$_2$Mo were calculated by using DFT in the theoretically optimized crystal structure in order to calculate elastic constants. The independent elastic constants were obtained from the set of lattice distortions and showing that Fe$_2$Mo is mechanically stable. The polycrystalline elastic parameters: bulk, shear and Young’s modules and Poisson’s ratio were determined from the single-crystal constants using the scheme of Voigt-Reuss-Hill approximation. Analysis of these data shows that the Fe$_2$Mo displays ductile behavior. The calculated elastic anisotropy shows that Fe$_2$Mo has isotropy elastic properties. Then, the Debye temperature and the anisotropic sound velocities of Fe$_2$Mo were calculated. The obtained results may also help to constrain future semi-empirical modeling or potentials for Fe$_2$Mo. Some results are reported for the first time and can be useful for further studies.

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