Investigation on properties of FeNi intermetallics under pressure by First-principles

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Abstract. In this paper, the structural stabilities, elastic, electronic and magnetic properties of three binary Fe-Ni intermetallics with different structure under pressure have been systematically investigated by first-principle method based on density functional theory. The results indicated that the lattice parameters and bulk modulus of Fe-Ni compounds at zero pressure match well with other experimental data and available theoretical calculated values. The calculated energy-volume and pressure-volume expressed that all the compounds are mechanical stability under pressure, and the volume variation increase with the increasing iron content under pressure. The shear deformation resistant and volume deformation resistant are estimated by elastic constant Cij and bulk modulus B. Meanwhile, applied pressure improved the ductility of the Fe-Ni compounds, elastic anisotropy of three compounds under pressure are arranged in the following order: Fe3Ni>FeNi>FeNi. Debye temperature ΘD of compounds gradually increase with the increase of iron contents and pressure, the temperature dependence of the linear thermal expansion coefficient α and heat capacity (Cv and Cp) are also calculated based on quasi-harmonic Debye model under pressure from 0 to 50GPa and various temperature. The results gain a better understanding of iron-nickel alloys.

1. Introduction
Iron-nickel alloy have shown great promise as anti-corrosion performance materials due to phase transition in structural and magnetic characteristics [1-2]. The iron-nickel alloys (FeNi3, FeNi and Fe3Ni) as one of temperature stability components of calibration equipment play an important role in aerospace, aeronautical and cryogenic engineering owing to their remarkable properties as well as high hardness and excellent ductility [3-5]. Moreover, FeNi3 have show outstanding magnetic [6-7] and thermal [8] properties, and the dispersion relation of FeNi3 have widely investigated by domestic and foreign references. Therefore, investigation on the Iron-nickel compounds has drawn extensive attention in many academic fields [9-11].

The fascinating properties of FeNi3, FeNi and Fe3Ni, such as chemical ordering in Ni rich Fe-Ni alloys and crystal structure transformation have draw extensively studied through theoretical simulation and experimental analysis [12]. The phonon dispersion relation of FeNi3 at 296K was obtained through inelastic scattering of slow neutrons by Hallman [13]. Moreover, experimental and theoretical methods were used to insight into the phonon dispersion relation of FeNi3 by S Garg and H C Sharma [14,15]. The FeNi have symmetric cubic structure seemingly, but in fact, it is tetragonal structure, which with small distortion [16]. Similarly, the electronic and magnetic structure of FeNi were targeted investigated considering as a cubic symmetry structure by Bohland Filho et al [17].
full phonon spectra of different structure of Fe$_3$Ni was investigated along the high symmetry directions of Brillouin zone [18]. Furthermore, the theoretical investigation for phonon dispersion relation of Fe-Ni alloys were implemented at room temperature compared with experimental reports [19]. Up to now, the structure and properties of Fe-Ni alloys were only investigated theoretically at 0 GPa by N Y pandya et al [20]. However, the formation and stability of thermodynamic conditions of the intermediate has not come to a report. And the structural, mechanical properties and thermodynamic properties of Fe-Ni compounds under the influence of temperature and pressure have not been investigated yet.

In this paper, the structural and mechanism properties of FeNi$_3$, FeNi and Fe$_3$Ni under various pressure from 0 to 50GPa were studied through first-principles calculation within the frame of Vienna ab initio simulation package code (VASP). The thermodynamic properties (Isothermal bulk modulus, Debye temperature, Linear thermal expansion coefficient and Heat capacity) were also investigated systematically based on temperature and pressure dependence of Fe-Ni compounds.

2. Computational details

In this paper, all the calculations are implemented in Vienna Ab-inito Simulation Package code(VASP) [21] based on the density functional theory (DFT) [22] method. To calculate the self-consistent electronic density, the generalized gradient approximation (GGA) [23] is preformed to obtain the exchange-correction function, which parametrized by the Perdew-Burke-Ernzerhof (PBE). To improve computational accuracy, the cutoff energy of atomic wave functions is set to be 500eV. Moreover, considering the k-mesh is forced to be centered on the gamma point, the Brillouin-zone sampling mesh for Monkhorst-Pack [24] k-point for FeNi$_3$, FeNi and Fe$_3$Ni are both set to be $13 \times 13 \times 13$. The energy and volume values were calculated when the atomic position relaxed sufficiently at each step. In addition, the convergence threshold of self-consistent field is $1.0 \times 10^{-5}$eV/atom, the $\sigma$ value of first-order Methfessel-Paxton smearing is 0.2eV.

3. Result and discussion

3.1. Structure properties

Figure 1 shown the optimized crystal structure, and table 1 tabulated the optimized crystal parameters at 0GPa of three Fe-Ni compounds together with the measured valued reported in the literature for comparison [25-27]. From table 1, the calculated crystal structure parameters are well matched with previous theoretical calculations and experimental data, which well verified the reasonability of Fe-Ni compounds models.

![Figure 1. The optimized crystal structures of Fe-Ni compounds (a) FeNi; (b) FeNi$_3$; (c)Fe$_3$Ni.](image)

**Table 1.** The calculated structure parameter of Fe-Ni compounds at 0 GPa, including lattice constant (Å), bulk modulus B (GPa), shear modulus G (GPa) and Young's modulus E (GPa).

| Phase | Composition (at% Ni) | space group | unitcell lattice parameter(Å) | $B_0$  | $G$   | $E$   | reference            |
|-------|----------------------|-------------|-------------------------------|-------|-------|-------|----------------------|
| FeNi$_3$ | 75              | Fm3m        | 3.547                         | 236.6 | 104.1 | 272.3 | This work             |
| FeNi | 50              | P4/mmm      | 3.475                         | 233.2 | 126   | 320.4 | This work             |
| FeNi$_3$ | 50              | Fm3m        | 3.545                         | 233.5 |       |       | cal[25-26]           |
Fe$_3$Ni & 25 & Fm3m & 3.556 & 241 & cal[27] \\

| Compound | Volume | Bulk Modulus | Energy Volume | This work |
|----------|--------|--------------|---------------|-----------|
| FeNi     | 3.589  | 167.1        | 114.7         | 280       |
| Fe       | 3.578  | 159.2        | This work     | cal[26]   |

Figure 2 shown the energy-volume E(V) data which obtained through the first principle calculation at a zero absolute temperature. Moreover, the E(V) curve are fitted to the Birch-Murnaghan model [28]:

$$E(V) = E_0 + \frac{9V_0B_0}{16} \left[ \left( \frac{V_0}{V} \right)^3 - 1 \right]^3 B_0 + \left[ \left( \frac{V_0}{V} \right)^2 - 1 \right]^2 \left[ 6 - 4 \left( \frac{V_0}{V} \right)^3 \right]$$

(1)

**Figure 2.** The function energy-volume of Fe-Ni compounds at a zero absolute temperature.

Where V0 is equilibrium volume, B0 and B’0 are bulk modulus and the first pressure derivative of bulk modulus, respectively.

$$B_0 = -V \left( \frac{dP}{dV} \right)_{P=0} = V_0 \left( \frac{d^2E(V)}{d^2V} \right)_{V_0}$$

$$B'_0 = \left( \frac{dP}{dV} \right)_{P=0}$$

(2)

Simultaneously, the function pressure-volume P(V) data has displayed in figure 3 to study the structural change with increasing pressure which in the range of 0-50GPa with a step of 10GPa. Meanwhile, the P(V) curves was calculated by the first principle with the equilibrium thermodynamic relation [29]:

$$P(V) = \frac{3}{2} B'_0 \left( \frac{V}{V_0} \right)^{-7/3} - \left( \frac{V}{V_0} \right)^{-5/3} + 1 + \frac{3}{4} \left( B'_0 - 4 \left( \frac{V}{V_0} \right)^{-2/3} \right)$$

(3)

**Figure 3.** The volume ratio V/V$_0$ of Fe-Ni compounds at different pressure with a step of 10GPa.
From figure 3, we can find that with the pressure increase, the volume ratio V/V₀ of all three Fe-Ni compounds presents a general decrease tendency. Moreover, the largest value of V/V₀ is Fe₃Ni, and the smallest value is FeNi₃ under the same pressure from 0 GPa to 50 GPa, which elucidating that the value change are ranged in the following order: Fe₃Ni < FeNi < FeNi₃. In other word, the most sensitive compounds of the effect of pressure to volume is FeNi₃, while the lowest is Fe₃Ni, which indicates that Fe₃Ni is harder to compress under pressure than that of other Fe-Ni compounds.

3.2. Mechanical properties

Elastic constants (Cᵢᵢ) of crystal obtained by non-volume-conserving method, plays an important role in characterizing mechanical and thermodynamic behaviors. Simultaneously, it is an imperative parameter include important elastic information concerning the response to various pressure. There are three (C₁₁, C₁₂ and C₄₄) independent elastic constants for the cubic crystal of Fe₃Ni and FeNi₃, six (C₁₁, C₁₂, C₃₃, C₃₅, C₄₄ and C₅₅) independent elastic constants for the tetragonal crystal of FeNi. The calculated elastic constants and elastic moduli of Fe-Ni compounds at 0 GPa are shown in Table 1, which are well match with the reference date. The mechanical stability criterion of cubic and tetragonal structure for Fe-Ni compounds are listed below:

For cubic (Fe₃Ni and FeNi₃) crystal [30]:

\[ C_{11} > 0, C_{44} > 0, C_{11} - C_{12} > 0, C_{11} + 2C_{12} > 0 \]

(4)

For tetragonal (FeNi) crystal [31]:

\[ C_{ij} > 0, i = 1 \sim 6, C_{11} + C_{33} > 2C_{13}, C_{11} > 2C_{12}, 2C_{11} + 2C_{12} + C_{33} + 4C_{13} > 0 \]

(5)

Figure 4 shows the calculated elastic constants for three Fe-Ni compounds under various pressure from 0 GPa to 50 GPa. From figure 4, we can clearly find that nearly all the elastic constants (Cᵢᵢ) growth linearly with the increasing pressure and all the Cij well meet the mechanical stability criterion when the pressure up to 50 GPa. Besides, C₁₁ is the largest elastic constant for all Fe-Ni compounds, which possibly indicates the higher deformation resistance in the direction of x-axis than other axis for the Fe-Ni compounds. Moreover, the value of C₄₄, C₅₅ and C₆₆ represent the ability to resist shear deformation [32]. From figure 4, we find that C₄₄ for Fe₃Ni is higher than other Fe-Ni compounds under the same pressure, which indicates the strongest ability to resist shear deformation.

![Figure 4](image-url)

**Figure 4.** The elastic constants of Fe-Ni compounds under various pressure.

Furthermore, once the elastic constants Cᵢᵢ was calculated, the bulk modulus B, shear modulus G and Young’s modulus E can be calculated by the Voigt-Reuss-Hill approximation (VRH) [33]. The computational equation are listed below [34-35]:

\[ B_{H} = \frac{1}{2} (B_{V} + B_{R}), \quad G_{H} = \frac{1}{2} (G_{V} + G_{R}), \quad E = \frac{9BG}{3B+G} \]

(6)

For a cubic crystal
The resistance of the figure (12) increases under the 0GPa pressure. The shear modulus at 0GPa increases with the increase of volume content. As the pressure rises, the deformation will become stronger. The Young’s modulus of Fe3Ni is higher than FeNi3. The 5, 10, 15, 20 volume indicates that the Fe-Ni compounds can show a high regularity of volume capacity. In this context, the Fe-Ni specimen presents a higher brittleness to deformation than the Fe-Ni specimen. Young moduli (5, 10, 15, 20) display a higher ratio of B/G. The figure (12) illustrates the transformation regularity of bulk modulus B, shear modulus G and Young’s modulus E for Fe-Ni compounds with the increasing pressure. The literature has highlighted that the bulk modulus B represent the volume change resistance, and the higher the B is, the better ability of resist deformation is [36]. As illustrated in figure 5, the B, G and E rise linearly with the increasing pressure, indicates that the resistance to volume deformation is stronger. In the meantime, one can clear see that the bulk modulus B increase with the increasing iron content of Fe-Ni compounds at a constant pressure ranges from 20-50GPa, which indicates that Fe3Ni has stronger capacity of the resist volume deformation under higher pressure. The ability of resist volume deformation of Fe3Ni under the pressure from 0GPa to 10GPa have a saltatorially increase. So the ability of resist volume deformation under the pressure from 20GPa to 50GPa complied with the following order: FeNi3 < FeNi < Fe3Ni. However, FeNi has stronger resistance to volume change at 0-20GPa, and the shear modulus G and Young’s modulus E is higher than FeNi3 likely.

\[ B_v = B_R = \frac{1}{3}(C_{11} + 2C_{12}) \quad (7) \]
\[ G_v = \frac{1}{5}(C_{11} + C_{12} + 3C_{44}) \quad (8) \]
\[ G_R = \frac{5C_{44}(C_{11} - C_{12})}{4C_{44} + 3(C_{11} - C_{12})} \quad (9) \]

For a tetragonal crystal
\[ B_v = \frac{2}{9}(C_{11} + C_{12}) + \frac{4}{9}C_{13} + C_{33} \quad (10) \]
\[ G_v = \frac{12(C_{44} + C_{66}) + C_{11} + C_{22} + 2C_{33} - 4C_{13}}{30} \quad (11) \]
\[ B_R = \frac{C_{33}(C_{11} + C_{12}) - 2C_{13}^2}{C_{11} + C_{12} + 2C_{33} - 4C_{13}} \quad (12) \]
\[ G_R = \frac{5C_{44}(C_{11} - 2C_{12})}{4C_{44} + 3(C_{11} - C_{12})} \quad (13) \]

Figure 5 displays the transformation regularity of bulk modulus B, shear modulus G and Young’s modulus E for Fe-Ni compounds with the increasing pressure. The literature has highlighted that the bulk modulus B represent the volume change resistance, and the higher the B is, the better ability of resist deformation is [36]. As illustrated in figure 5, the B, G and E rise linearly with the increasing pressure, indicates that the resistance to volume deformation is stronger. In the meantime, one can clear see that the bulk modulus B increase with the increasing iron content of Fe-Ni compounds at a constant pressure ranges from 20-50GPa, which indicates that Fe3Ni has stronger capacity of the resist volume deformation under higher pressure. The ability of resist volume deformation of Fe3Ni under the pressure from 0GPa to 10GPa have a saltatorially increase. So the ability of resist volume deformation under the pressure from 20GPa to 50GPa complied with the following order: FeNi3 < FeNi < Fe3Ni. However, FeNi has stronger resistance to volume change at 0-20GPa, and the shear modulus G and Young’s modulus E is higher than FeNi3 likely.

Figure 5. The pressure dependence of bulk modulus B, shear modulus G and Young’s modulus E for Fe-Ni compounds.

Generally speaking, previous studies has investigated that the B/G ratio and \( \nu \) determined the ductility and brittle of the Fe-Ni compounds [37,38]. The pressure dependence of B/G ratio and Poisson’s ratio of the Fe-Ni compound are presented in figure 6. The Poisson’s ratio \( \nu \) can be calculated:
Figure 6. The variation of B/G ratio and poisson’s ratio \( \nu \) with the various pressure.

The critical value of the B/G ratio and \( \nu \) to estimate the ductility of materials are 1.75 and 0.26, respectively. From figure 6, we can find that the B/G ratio and \( \nu \) of FeNi3 and FeNi are both greater than 1.75 and 0.26 respectively, which signifies a ductile behavior. However, the B/G ratio and \( \nu \) of Fe3Ni is 1.76 and 0.27 at 40GPa, which signifies that Fe3Ni shows a ductile behavior in 40-50GPa, and a brittle behavior in 0-40GPa, which illustrate that the brittle behavior turn into ductile behavior when the pressure up to 40GPa. Furthermore, all the B/G ratio and \( \nu \) exhibit a increasing tendency with rising pressure,indicating that the applied pressure can improve the ductility of the Fe-Ni compounds.

Figure 7. The variation of microhardness with the various pressure.

The microhardness \( H \) of Fe-Ni compounds is anther significant parameter to estimated the mechanical properties of materials, it can be evaluated by B, G and E. In this work, Yousef's empirical formula is adopted to predict the microhardness \( H \) \cite{39}:

\[
H = \frac{(1-2\nu)E}{6(1+\nu)} = \frac{G* E}{9B}
\]
Figure 7 displays the pressure dependence of microhardness for considered compounds. It is found that the microhardness of Fe-Ni compounds improved by the rising external pressure, and the value of microhardness of the considered compounds ranked in the following descending order: Fe$_3$Ni > FeNi > FeNi$_3$, which matches well with the result of brittleness. Otherwise, compared with figure 5, the influence of shear modulus $G$ and Young’s modulus $E$ to the microhardness is stronger than that of bulk modulus $B$.

In this work, the elastic anisotropy was calculated by ranganathan’s formula as below [40], which displayed in table 2. From table 2, we can find that all the Fe-Ni compounds are anisotropic materials due to AU > 0, and the value AU of all three Fe-Ni compounds increased with the applied rising pressure, which indicates the enhanced anisotropy of Fe-Ni compounds under applied pressure. Moreover FeNi$_3$ occupied the biggest anisotropy and impact on anisotropy with the rising external pressure, and the anisotropy sequence under applied pressure from high to low ranked in the follow order: FeNi$_3$ > FeNi > Fe$_3$Ni.

$$A^U = 5\frac{G_V}{G_R} + \frac{B_L}{B_R} - 6$$

(16)

| Universal anisotropy | Pressure(GPa) | FeNi$_3$ | FeNi | Fe$_3$Ni |
|----------------------|--------------|---------|------|---------|
| AU (GPa)             | 0            | 1.163   | 0.692| 0.334   |
|                      | 10           | 1.239   | 0.706| 0.473   |
|                      | 20           | 1.268   | 0.742| 0.541   |
|                      | 30           | 1.316   | 0.801| 0.553   |
|                      | 40           | 1.477   | 0.815| 0.559   |
|                      | 50           | 1.587   | 0.868| 0.689   |

3.3. Thermodynamic properties

In order to have a further study of thermodynamic behaviors of Fe-Ni compounds under pressure, the quasi-harmonic Debye model is employed to calculate the Debye temperature $\Theta_D$, heat capacity $C_v$, $C_p$, bulk modulus $B$ and linear thermal expansion coefficient of Fe-Ni compounds. To calculate these thermodynamic properties, the obtained $E(V)$ data in section 3.1 was employed into Gibbs program, which match with non-equilibrium Gibbs function $G^*(V; P; T)$[41-42]. The energy-volume calculations conclude 21 volumes point from 0.80a to 1.20a with an interval of 0.02a, which improved the precision of the calculation of thermodynamic behaviors.

The variation of debye temperature of three Fe-Ni compounds at different temperature and pressure are shown in figure 8. what can be clearly seen in this figure is the phenomenal growth of Debye temperature at the fixed temperature with the increasing pressure, and nearly keep a constant from 0 to 200K and linearly decrease from 200 to 1400K. The variation tendency of linear thermal expansion coefficient $\alpha$ of Fe-Ni compounds with different temperature and pressure are shown in figure 9. What stands out in figure 9 is the same increase tendency of linear thermal expansion coefficient $\alpha$ for three Fe-Ni compounds. Furthermore, it is shown that the $\alpha$ is linear with T3 in the ranging from 0 to 300K, which suggest a rapid increasing with the temperature increase.
Figure 8. The pressure and temperature dependences of Debye temperature for Fe-Ni compounds.

Figure 9. The pressure and temperature dependences of linear thermal expansion coefficient for Fe-Ni compounds.

Figure 10 and 11 shows a significant thermodynamic parameter of heat capacity which conclude isochoric heat capacity(CV)and isobaric heat capacity (CP). From the variation tendency of CV and CP with different temperature and pressure,it is clear show that there has been a marked rise in the number of CV and CP when temperature is below 300K, which subordinated to Debye's law. Otherwise, the CP is anticipated to continue increasing, while CV is likely to remain a constant, possibly due to the CV followed the Dulong-Petit limit under higher temperature. Moreover, the pressure is a complicating factor for the heat capacity, the higher the pressure, the lower the heat capacity.
Figure 10. The pressure and temperature dependences of $C_V$ for Fe-Ni compounds.

Figure 11. The pressure and temperature dependences of $C_P$ for Fe-Ni compounds.

4. Conclusion
We investigated the properties of Fe-Ni compounds using first principle method, the main conclusions are summed up as follows:

1) The calculated results of lattice parameters based on density-functional theory (DFT) are well matched with experiment and theoretical dates. The value of $V/V_0$ decrease with rising pressure and increase with increasing iron content.

2) The three Fe-Ni binary compounds are mechanical stability under pressure from 0 to 50GPa. Appropriate pressure can improve bulk modulus B, shear modulus G, and Young’s modulus E of FeNi$_3$, FeNi and Fe$_3$Ni, and they ranked in the follow order: FeNi$_3$ < FeNi < Fe$_3$Ni. The ductility of FeNi and FeNi$_3$ enhance with increasing pressure, but there has a ductile conversion behavior at 30GPa for Fe$_3$Ni.

3) The microhardness of three Fe-Ni binary compounds improved by the rising pressure, and the value of microhardness of Fe-Ni compounds ranked as: FeNi$_3$ < FeNi < Fe$_3$Ni under the same pressure. On the contrary, the value of elastic anisotropy can be arranged as opposite order: Fe$_3$Ni < FeNi < FeNi$_3$ compared with microhardness.
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