

Article

A First-Principles Study of the Structural, Elastic, and Mechanical Characteristics of Mg₂Ni Subjected to Pressure Conditions

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Abstract: This study employs first-principles calculations to examine structural, elastic, and mechanistic relationships of Mg₂Ni alloys under varying conditions of pressure. The investigation encompasses Young's modulus, bulk modulus, shear modulus, Poisson's ratio, and anisotropy index, as well as sound velocity, Debye temperature, and related properties. Our findings indicate that the lattice parameters of Mg₂Ni in its ground state are in agreement with values obtained experimentally and from the literature, confirming the reliability of the calculated results. Furthermore, a gradual decrease in the values of the lattice parameters a/a_0 and c/c_0 is observed with increasing pressure. Specifically, the values for C_{13} and C_{33} decrease at a hydrostatic pressure of 5 GPa, while C_{11} and C_{13} increase when the external hydrostatic pressure exceeds 5 GPa. All other elastic constants exhibit a consistent increasing trend with increasing pressure between 0 and 30 GPa, with C_{11} and C_{12} increasing at a faster rate than C_{44} and C_{66} . In the 0–30 GPa pressure range, Mg₂Ni satisfies the mechanical stability criterion, indicating its stable existence under these conditions. Additionally, the Poisson's ratio of Mg₂Ni consistently exceeds 0.26 over a range of pressures from 0 to 30 GPa, signifying ductility and demonstrating consistency with the value of B/G . The hardness of Mg₂Ni increases within the pressure range of 0–5 GPa, but decreases above 5 GPa. Notably, the shear anisotropy of Mg₂Ni exhibits greater significance than the compressive anisotropy, with its anisotropy intensifying under higher pressures. Both the sound anisotropy and the Debye temperature of Mg₂Ni demonstrate an increasing trend with rising pressure.

Keywords: Mg₂Ni; elastic constants; mechanical properties; first-principles calculations

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1. Introduction

The escalating global appetite for renewable and clean energy has prompted significant interest in hydrogen energy as a clean and efficient energy carrier. Nevertheless, the storage and transportation of hydrogen present key challenges that impede its widespread application. Consequently, hydrogen storage alloys based on Mg have emerged as a prominent focus in hydrogen storage research due to their high hydrogen capacity and reversible hydrogen adsorption and desorption properties [1,2]. Mg₂Ni, as a representative of hydrogen storage materials based on Mg [3], exhibits a high theoretical capacity for hydrogen storage and favorable hydrogen adsorption/desorption kinetics. Additionally, it is non-polluting, showcases good reversibility, is cost-effective, and benefits from ample crustal reserves. Consequently, it has garnered significant attention from researchers [4–8]. Skryabina et al. employed a rapid forging plastic deformation technique to process synthesized Mg/Ni fine-powder mixtures, revealing that the quantity of Mg₂Ni alloy synthesized directly increases proportionally with temperature above a certain threshold [9]. Guo et al. discussed the precipitation behavior of nanocrystalline LaH₃ and Mg₂Ni, observing a significant enhancement in the dehydrogenation performance of in situ-formed Mg₂Ni-LaH₃ nanocomposites.

The formation of LaH_3 facilitates the hydrogenation process, while Mg_2Ni contributes to improved dehydrogenation performance [10]. Gao et al. investigated the thermal stability, electronic properties, and hydrogen adsorption/desorption on a $\text{Mg}_2\text{Ni}(010)$ surface with rare-earth (Y, Ce, La, Sc) doping using first-principles calculations. The rare-earth atoms weaken the binding strength between H and the $\text{Mg}_2\text{Ni}(010)$ substrate, thereby reducing the diffusion and desorption energy barriers of hydrogen and enhancing the hydrogen storage performance of Mg_2Ni . Among the four rare-earth elements studied, Ce exhibits the most promising potential [11]. In the realm of catalysis, Mg-based alloys exhibit promising potential [12,13]. For instance, the anticipated application of Mg_2Ni in catalysts is underscored by its exceptional hydrogen adsorption/desorption properties, which offer broad prospects for its utilization in hydrogen chemical reactions [14]. Furthermore, with the advancement of materials science and engineering, research on the performance of hydrogen storage alloys under extreme conditions, such as high pressure, has garnered increasing attention. Chen et al. measured the resistance of MgNi and MgNH powders under compressive conditions up to 6 gigapascals (GPa) using the 2 2 4 four-point probe method at 208 °C. In addition, the effects of high-pressure treatment and heating at 4008 °C (with or without the hydrogen source LiAlH_4) were investigated [15]. Under high-pressure environments, the crystal structure, elasticity, and mechanical properties of materials undergo significant changes, presenting new challenges for material application and performance design [16,17]. Thus, an in-depth exploration of the properties of Mg_2Ni under high-pressure conditions can not only furnish theoretical support for its application in hydrogen storage and catalysis but also facilitate the advancement of material property design and optimization under extreme conditions.

The first-principles calculation method is characterized by its precision and wide applicability, finding extensive utilization in the fields of materials science, condensed matter physics, and chemistry. This approach enables an in-depth understanding of the microscopic structure and properties of materials, offering crucial theoretical support for the design of new materials and the investigation of catalytic mechanisms [18–24]. The aim of this work is to comprehensively investigate the structure, elasticity, and mechanical behavior of Mg_2Ni at different pressures using first-principles calculations, with the objective of offering theoretical support for taking into account its properties in practical applications. Initially, the crystal structure alterations of Mg_2Ni under different pressure conditions were scrutinized, encompassing lattice parameters, interatomic distances, and other pertinent factors, employing density functional theory (DFT) calculations. Subsequently, the elastic properties of Mg_2Ni under diverse pressures, including elastic constants, shear modulus, and related aspects, were delved into to discern the material's elastic response. Lastly, the mechanical properties of Mg_2Ni under varying pressures, such as the stress–strain relationship and material deformation behavior, were explored to obtain a comprehensive understanding of the structural and property modifications of Mg_2Ni under pressure. By conducting an in-depth exploration of these properties of Mg_2Ni , we can gain enhanced insights into its behavior under high-pressure environments and furnish a reference for designing new high-performance materials. This study will furnish theoretical backing for the application of metal hydride materials under high-pressure conditions and is poised to introduce fresh ideas and methodologies for the future design and engineering of materials.

2. Calculation Details

2.1. First-Principles Calculations

This study uses density functional theory (DFT) [25,26] implemented in the Cambridge Serial Total Energy Package (CASTEP) code [27–29] for calculations. Specifically, the energy functional of exchange correlation is described using the Perdew–Burke–Ernzerh (PBE) generalized gradient approximation method [30], which demonstrates favorable accuracy in elucidating the electronic interactions within the material. The Broyden–Fletcher–Goldfarb–Shanno (BFGS) [31] algorithm is used to relax all atomic positions and lattice parameters based on overall force and energy. Tolerances for convergence were set

as follows: energy deviation less than 5.0×10^{-6} eV/atom, ionic force less than 0.03 eV/Å, stress deviation less than 0.02 GPa, maximal inter-cycle shift less than 5×10^{-4} Å, and the description of ion–electron interactions uses the ultrasoft pseudopotential (USPP) [32]. Mg and Ni have $2p^6 3s^2$ and $3s^2 3p^1$ electron valence configurations. The cut-off energy for the plane wave is 600 eV, with an energy convergence of 1.0×10^{-6} eV/atom. A Brillouin zone sampling k-point grid was generated using the Monkhorst–Pack scheme with an $11 \times 11 \times 13$ k-point grid [33]. Before the elastic constants were calculated for Mg_2Ni intermetallic compounds under pressure, the compounds under pressure were optimized by full relaxation in shape, volume, and position of the atoms till the interatomic forces became smaller than 1.0×10^{-2} eV/Å. Then, the elastic constants were calculated for Mg_2Ni intermetallic compounds under pressure.

2.2. Calculation of Elastic Constants

The atomic structure of Mg_2Ni exhibits a hexagonal crystal system (as depicted in Figure 1) with highly symmetric D_{6h}^4 , characterized by lattice parameters $a = 5.219$, $c = 13.293$ [34] and space group P6222 (No. 180) [35]. There are 6 Ni atoms and 12 Mg atoms in each protocell, which can be partitioned into 6 levels parallel to the xy plane. Within each Mg layer, two Ni atoms fill the 3d and 3b positions, while within each Ni layer, four Mg atoms fill the 6i and 6f positions, respectively.

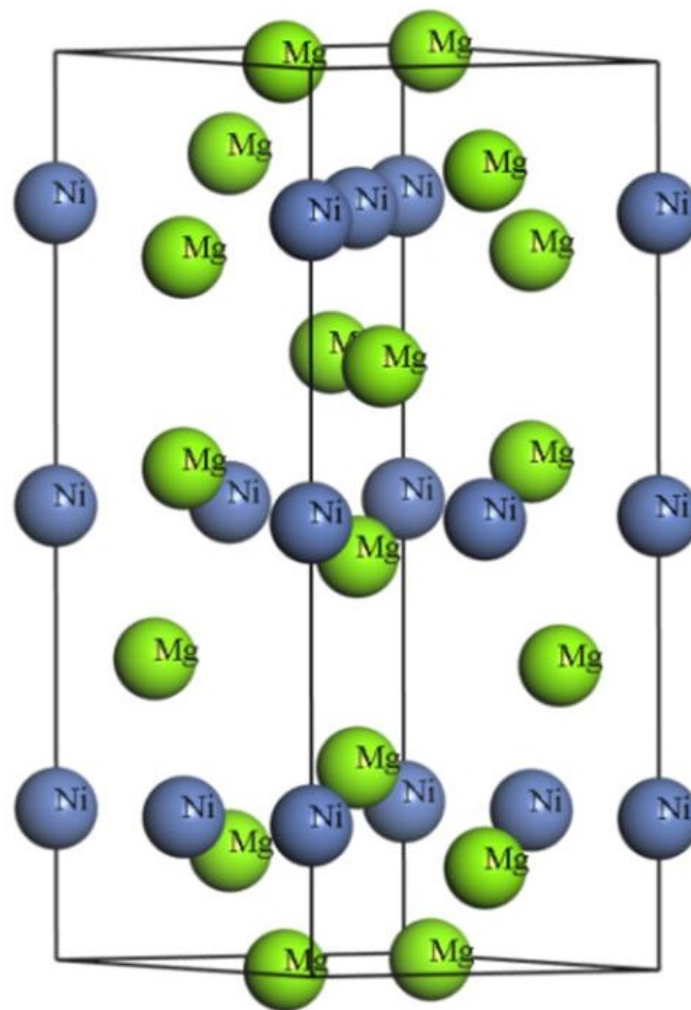


Figure 1. The single-cell model of Mg_2Ni .

The hexagonal intermetallic compound Mg_2Ni has six independent single-crystal constants of elasticity, designated C_{11} , C_{12} , C_{13} , C_{33} , C_{44} , and C_{66} . In the investigation,

we ascertain all elastic constants from optimized single cells at various pressures using the strain–stress relationship method. The constants of elasticity are determined from first-order derivatives with the tensors of stress and strain. The stress tensor is obtained by carrying out 6 final deformations on grid and deriving the strain constants using the strain–stress relationship [36]. When calculating the elastic tensor for ions that are rigid, ion relaxation is also taken into consideration. The ion contribution is obtained by the inverse of the ion Hessian matrix and multiplication by the internal tensor of strain [37]. The ultimate elastic constants encompass both the contribution of rigid ion deformation and ion relaxation.

3. Results and Discussion

3.1. High-Pressure Structural Properties

After geometric structure optimization, the optimal structural model of Mg_2Ni was obtained, with the corresponding parameters of $a = 5.218 \text{ \AA}$ and $c = 13.249 \text{ \AA}$. Experimental work by K. Yvon [34] determined the cell parameters of Mg_2Ni to be $a = 5.219 \text{ \AA}$ and $c = 13.293 \text{ \AA}$, while theoretically, Liu et al. [38] obtained $a = 5.217 \text{ \AA}$ and $c = 13.276 \text{ \AA}$ for the cell parameters of Mg_2Ni . Upon comparison, the cell parameters derived from this computation were found to be in good agreement with existing theoretical and experimental values, indicating the correctness within our computational method.

The structure of the cell was optimized, the pressure range was 0 to 30 GPa, and corresponding structural parameters at each pressure were obtained. The variation in the Mg_2Ni cell's a/a_0 , c/c_0 and cell volume V/V_0 as a function of pressure is presented in Figure 2. The values of parameters a/a_0 and c/c_0 gradually decrease as pressure increases, as the crystal cell experiences external forces under pressure, leading to a reduction in the distance between atoms and a subsequent decrease in the a/a_0 and c/c_0 parameters. Consequently, as pressure increases, volume V also decreases.

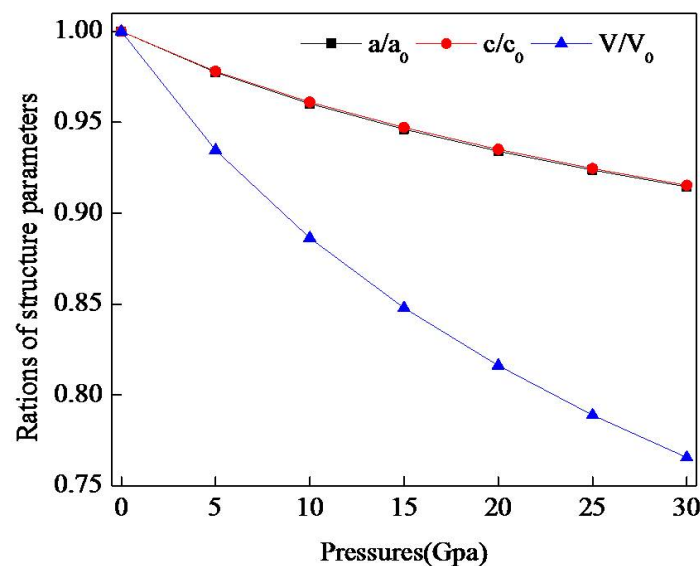


Figure 2. Pressure-dependent ratio of structural parameters in Mg_2Ni .

We performed polynomial fitting of a/a_0 , c/c_0 , and V/V_0 with respect to pressure, yielding an equation that describes their relationship, as depicted in Equation (1). In this equation, the constant term closely approximates the value 1, indicating a favorable fit.

$$\begin{aligned}
 a/a_0 &= 0.99988 - 4.8900 \times 10^{-3}P + 1.0483 \times 10^{-4}P^2 - 1.2263 \times 10^{-6}P^3 \\
 c/c_0 &= 0.99986 - 4.7500 \times 10^{-3}P + 9.87698 \times 10^{-5}P^2 - 1.14188 \times 10^{-6}P^3 \\
 V/V_0 &= 0.99955 - 1.435 \times 10^{-3}P + 3.40549 \times 10^{-4}P^2 - 4.09107 \times 10^{-6}P^3
 \end{aligned} \quad (1)$$

The elastic constants are physical properties that characterize the relation between strain and stress in anisotropic media, and are essential for understanding the elastic behavior of materials. Mg₂Ni, with its hexagonal crystal structure, has five independently determined constants of elasticity: C_{11} , C_{12} , C_{13} , C_{33} , and C_{44} . Additionally, it exhibits the relationship $C_{66} = (C_{11} - C_{12})/2$. Among these constants, the strain response of the crystals to tensile stress along the crystal axes [100] and [001] directions, respectively, is described by C_{11} and C_{33} . C_{44} reflects the [100] direction shearing strength of the crystals, while C_{66} reflects the [001] direction shearing strength. The C_{12} and C_{13} elastic constants are associated with elastic deformation. Upon applying hydrostatic pressure of 5 GPa, we observed a decrease in the values of C_{13} and C_{33} , while the values of C_{11} and C_{13} increased with further increase in pressure. All other elastic constants exhibited a monotonic increase as pressure varied from 0 to 30 GPa, with the growth rate for C_{11} and C_{12} surpassing that of C_{44} and C_{66} . The alterations in the interactions between atoms within the crystals under hydrostatic pressure led to changes in the elastic constants. The elastic constants of Mg₂Ni at pressures from 0–30 GPa are given in Table 1.

Table 1. Elastic constants of Mg₂Ni at various pressures (C_{ij} in GPa).

Pressure	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	C_{66}
0	115.857	44.723	74.463	190.004	21.289	35.567
5	144.622	61.676	50.827	162.876	24.762	41.473
10	174.032	80.436	61.925	182.278	27.401	46.798
15	196.713	93.473	72.256	207.105	28.764	51.620
20	210.861	99.683	88.357	240.581	30.569	55.589
25	243.136	121.670	96.967	252.583	31.446	60.733
30	284.700	156.732	134.682	300.764	31.681	63.984

The variations in C_{11} , C_{12} , C_{13} , and C_{33} under different hydrostatic pressures are influenced by the lattice structure and interatomic interactions, resulting in distinct trends. Furthermore, the relatively weak response of crystal shear properties to pressure is reflected in the slower growth rate of C_{44} and C_{66} , which represent the responsiveness of crystals to shear stresses. It is noteworthy that C_{11} remains consistently lower than C_{33} under equivalent pressure, indicating compression in the [100] direction is easier than in the [001] dimension. In addition, for crystals of hexagonal shape, the condition of mechanical stability in isotropic pressure is given in Equation (2) [39,40].

$$\tilde{C}_{44} > 0, \tilde{C}_{11} - |\tilde{C}_{12}| > 0, \tilde{C}_{33}(\tilde{C}_{11} + \tilde{C}_{12}) - 2\tilde{C}_{13}^2 > 0 \quad (2)$$

where $\tilde{C}_{ii} = C_{ii} - P$ ($i = 1, 3, 4$), $\tilde{C}_{12} = C_{12} + P$, $\tilde{C}_{13} = C_{13} + P$.

The different crystal deformations under hydrostatic pressure are related to the different criterion conditions. Parameters $\tilde{C}_{44}$ and $\tilde{C}_{66}$ signify shear deformation of crystal cells under hydrostatic pressure, while $\tilde{C}_{11} - |\tilde{C}_{12}|$ represents the expansion along the main axis and the contraction along the perpendicular main axis. Parameter $\tilde{C}_{33}(\tilde{C}_{11} + \tilde{C}_{12}) - 2\tilde{C}_{13}^2$ indicates the volumetric deformation under pressure. It is evident that Mg₂Ni fulfills the mechanical stability criterion ranges from 0 GPa to 30 GPa, indicating its stable existence under pressures within this range.

3.2. Mechanical Properties under Pressure

In industrial applications, macromechanical parameters like crystal shear modulus, bulk modulus, Young's modulus, Poisson's ratio, etc., are valuable for elucidating macromechanical properties of crystals. Commonly used methods for determining the shear modulus, Young's modulus, and bulk modulus through elastic constants include Reuss approximation and Voigt approximation. The Reuss approximation uses uniform stress distribution to establish the minimum true shear modulus and bulk modulus for the polycrystal, while

Voigt's approximation uses uniform strain distribution within the polycrystalline structure to establish the maximum true shear modulus and bulk modulus for the polycrystal. Hill proposed that taking the average of the two is more realistic, known as the Voigt–Reuss–Hill approximation method [41]. This approach calculates the crystal bulk modulus and shear modulus as average values of the Voigt and Reuss bulk moduli (BV, BR) and shear moduli (GV, GR), respectively. For hexagonal crystal systems, the Voigt and Reuss bulk moduli (BV, BR) and shear moduli (GV, GR) are defined as Equation (3) [42,43].

$$\begin{aligned} B_V &= \frac{2C_{11} + 2C_{12} + 4C_{13} + C_{33}}{9} & G_V &= \frac{C_{11} + C_{12} - 4C_{13} + 2C_{33} + 12C_{44} + 12C_{66}}{30} \\ B_R &= \frac{(C_{11} + C_{12})C_{33} - 2C_{13}^2}{C_{11} + C_{12} - 4C_{13} + 2C_{33}} & G_R &= \frac{5[(C_{11} + C_{12})C_{33} - 2C_{13}^2]C_{44}C_{66}}{6B_VC_{44}C_{66} + 2[(C_{11} + C_{12})C_{33} - 2C_{13}^2](C_{44} + C_{66})} \end{aligned} \quad (3)$$

where $C_{66} = (C_{11} - C_{12})/2$. Upon calculating the BV and GV using Voigt's labeling, BR and GR using Reuss's labeling, the bulk modulus (B), shear modulus (G), Young's modulus (E), and Poisson's ratio (ν) were subsequently determined for different pressures of respective precipitation phases according to Equation (4).

$$B = \frac{B_V + B_R}{2} \quad G = \frac{G_V + G_R}{2} \quad E = \frac{9BG}{3B + G} \quad \nu = \frac{3B - 2G}{6B + 2G} \quad (4)$$

The relationship between shear modulus, bulk modulus, and Young's modulus of the Mg_2Ni intermetallic compound depending on pressure is illustrated in Figure 3. The shear modulus reflects resistance of the material to shear deformation under stress, while the bulk modulus indicates deformation resistance under applied stress, with higher values representing greater resistance. Young's modulus characterizes the material's stiffness, with larger values indicating greater stiffness. As depicted in Figure 3, it is evident that Young's modulus (E), the shear modulus (G), and the bulk modulus (B) increase monotonically with increasing pressure. This behavior can be attributed to the symmetry of Mg_2Ni 's hexagonal crystal system. The increase in external pressure alters the interatomic interactions within the lattice, consequently leading to an increase in the bulk, shear, and Young's moduli of the crystals.

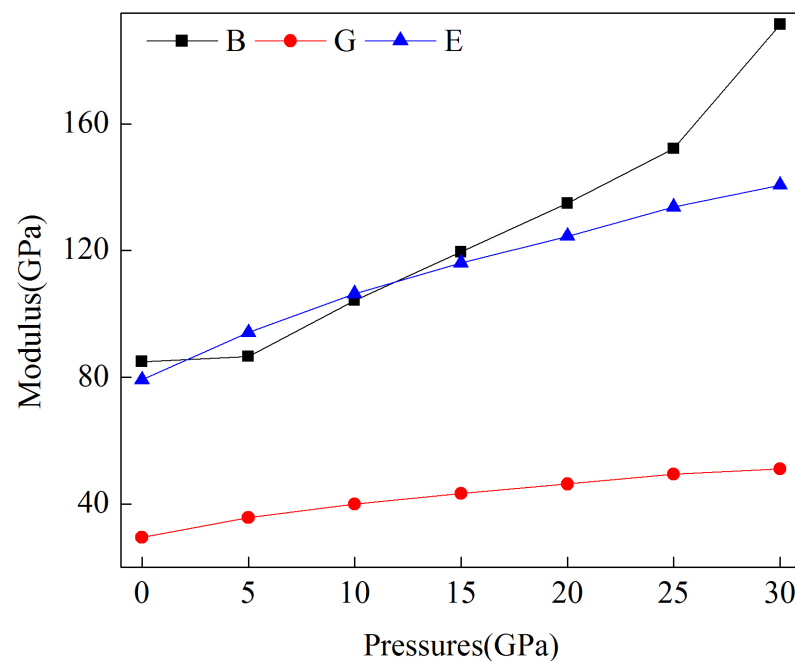


Figure 3. The bulk modulus (B), shear modulus (G), and Young's modulus (E) of Mg_2Ni at different pressures.

The B/G value indicates the ductility and brittleness of a material according to the Pugh rule [44]. B/G is a measure of ductility, with materials demonstrating ductile behavior when $B/G > 1.75$ and brittle behavior when $B/G < 1.75$. Figure 4a presents the B/G ratio of the Mg_2Ni alloy. Within the 0–5 GPa pressure range, the B/G value exhibits a decreasing trend, reaching 2.423 GPa at 5 GPa of applied hydrostatic pressure. Beyond 5 GPa, the B/G value increases with rising pressure, consistently exceeding 1.75 within the 0–30 GPa pressure range, indicating ductile behavior. Additionally, within the 0–5 GPa range, the ductility demonstrates a decreasing trend, while it increases with rising pressure beyond 5 GPa. In accordance with the rule of Frantsevich et al. [45], materials primarily exhibit brittle behavior when the Poisson's ratio (ν) is $\nu < 0.26$, and conversely, ductile behavior when $\nu > 0.26$. Figure 4b illustrates the dependence of Poisson's ratio (ν) on pressure for the Mg_2Ni alloy. Within the 0–5 GPa pressure range, the ν demonstrates a decreasing trend, reaching 0.3186 under an external hydrostatic pressure of 5 GPa. Beyond 5 GPa, the Poisson's ratio increases with rising pressure, consistently exceeding 0.26 within the 0–30 GPa pressure range, indicating ductile behavior. These findings align with the observed B/G value consistency.

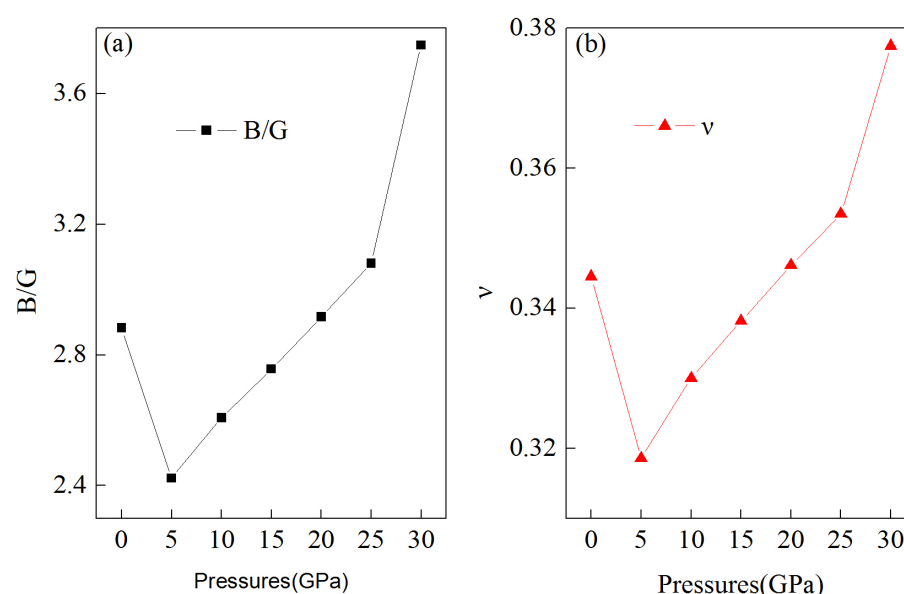


Figure 4. (a) Variation curves of G/B modulus and (b) Poisson's ratio (ν) with pressure for Mg_2Ni .

For the hexagonal crystal structure, the Cauchy pressure on the (100) face is denoted as $(C_{13} - C_{44})$, while on the (001) face it is represented as $(C_{12} - C_{66})$. In accordance with Pettifor's rule [46], a higher Cauchy pressure value indicates a greater number of metallic bonds within the metal, correlating with increased toughness. Conversely, a higher negative value of Cauchy pressure suggests a greater number of covalent bonds, indicating increased brittleness. As illustrated in Figure 5, the Cauchy pressure $(C_{12} - C_{66})$ exhibits an increasing trend with rising pressure, whereas the Cauchy pressure $(C_{13} - C_{44})$ demonstrates a decreasing trend within the 0–5 GPa range. Beyond 5 GPa, $C_{13} - C_{44}$ increases with rising pressure. Within the 0–30 GPa pressure range, both $C_{12} - C_{66}$ and $C_{13} - C_{44}$ are positive, signifying a prevalence of metallic bonding on the surface of the Mg_2Ni alloy. Additionally, at equivalent pressures, the $(C_{12} - C_{66})$ Cauchy pressure remains consistently lower than the corresponding $(C_{13} - C_{44})$ Cauchy pressure, indicating that the (100) surface's bonding alloy property is of greater significance than that of the (001) surface.

Hardness provides a measurement of a material's ability to resist deformation, whether elastic or plastic, or damage when subjected to external forces. These properties are influenced by factors such as the material's elastic constants, plastic behavior, strain, ductility,

and strength. In theory, Equation (5) can be used to estimate the hardness (H) of a polycrystalline material [47].

$$H = 2 \left(\frac{G^3}{B^2} \right)^{0.585} - 3 \quad (5)$$

Figure 6 shows the hardness of Mg_2Ni at different pressures. It is a fact that at pressures ranging from 0 to 5 GPa, the hardness increases proportionally with the rise in pressure. However, when the pressure exceeds 5 GPa, with increasing pressure, hardness tends to decrease.

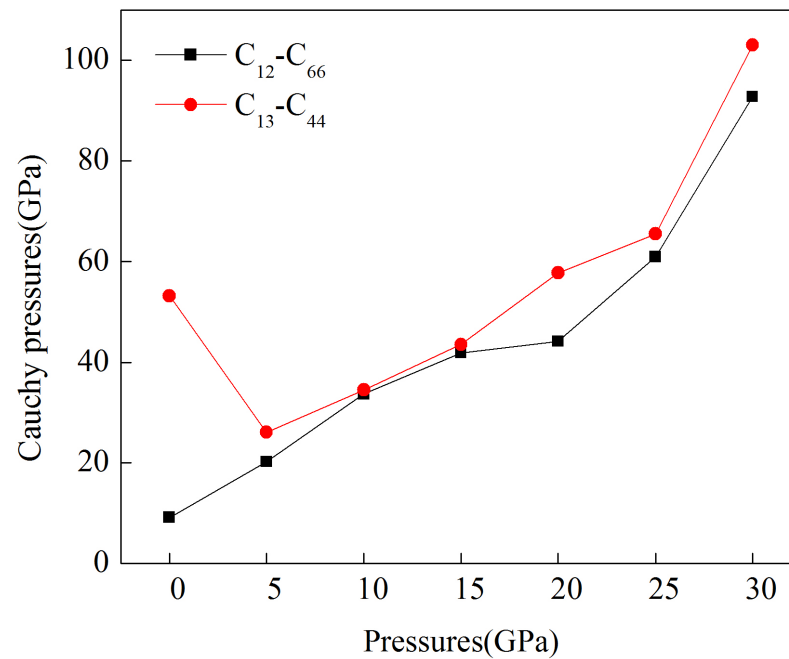


Figure 5. Cauchy pressure of the Mg_2Ni alloy under varying pressures.

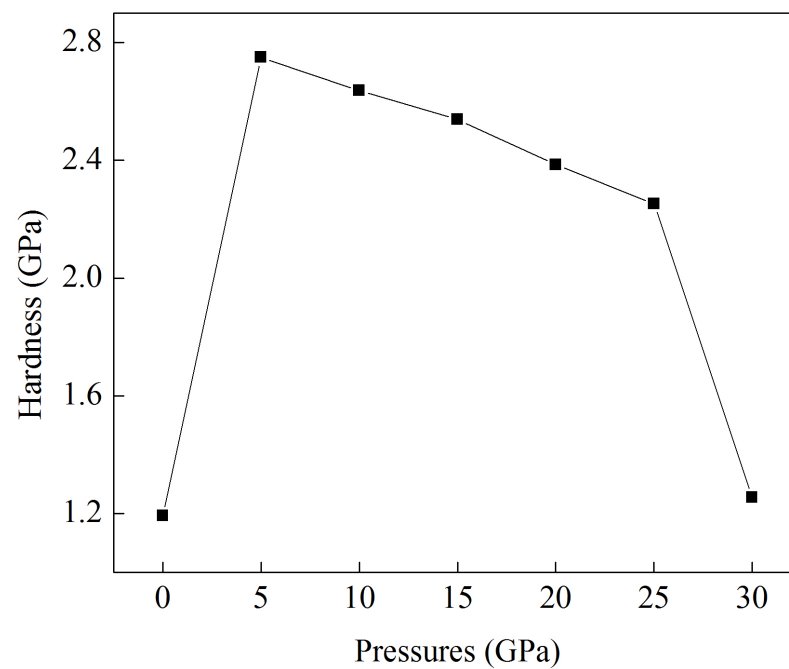


Figure 6. Hardness of Mg_2Ni alloys under different pressure conditions.

3.3. Elastic Anisotropy under Pressure

In materials science, the directional dependency in material physical properties is referred to as elastic anisotropy, a phenomenon commonly observed in most materials. The investigation of elastic anisotropy in intermetallic compounds is closely associated with the microfracture behavior of materials. The elastic anisotropy factor serves to quantify the variation in shear deformation energy across different directions, and therefore, helps to understand how a material resists shearing in different orientations. Specifically, $A_{\{100\}}$ denotes the shearing anisotropy coefficient between the (100) shear planes and the $\langle 011 \rangle$ and $\langle 010 \rangle$ orientations, reflecting shear deformation along these directions on the (100) surface. Similarly, $A_{\{010\}}$ represents the factor of shear anisotropy between (010) shear planes and the $\langle 101 \rangle$ and $\langle 001 \rangle$ orientations, characterizing shear deformation along these directions on the (010) surface. Lastly, $A_{\{001\}}$ denotes the factor of shear isotropy between the (001) plane of shear and the $\langle 110 \rangle$ and $\langle 010 \rangle$ orientations, illustrating shear deformation along these directions on the (001) surface. For isotropic materials, the values of $A_{\{100\}}$, $A_{\{010\}}$, $A_{\{001\}}$ are expected to be 1, with deviations from this value indicating the degree of anisotropy.

The elastic constants obtained provide the basis for further calculation of elastic anisotropy factors, which are presented in the following equations [48]:

$$A_{\{100\}} = \frac{4C_{44}}{C_{11} + C_{33} - 2C_{13}} \quad A_{\{010\}} = \frac{4C_{55}}{C_{22} + C_{33} - 2C_{23}} \quad A_{\{001\}} = \frac{4C_{66}}{C_{11} + C_{22} - 2C_{12}} \quad (6)$$

Figure 7a shows the $A_{\{100\}}$, $A_{\{010\}}$, and $A_{\{001\}}$ anisotropy factors at various pressures for Mg₂Ni. It is evident from the figure that $A_{\{100\}}$ and $A_{\{010\}}$ are considerably less than 1 and exhibit a monotonically decreasing trend with increasing pressure, while the value of $A_{\{001\}}$ remains constant at 1 across different pressures. These findings suggest an increase in anisotropy of Mg₂Ni in the {100} and {010} planes with increasing pressure, whereas the compound demonstrates isotropy in the {001} plane. Given that Mg₂Ni belongs to the hexagonal crystal system, the {100} and {010} planes in its structure possess lower symmetry, leading to stronger anisotropy of the material's elastic properties in these planes. Conversely, the {100} plane exhibits higher symmetry, resulting in isotropic elastic properties. Therefore, the observed increase in {100}- and {010}-plane anisotropy and {001}-plane isotropy in Mg₂Ni is consistent with the general characteristics of hexagonal crystallographic materials.

The compressive anisotropy factor (A^B) and shear anisotropy factor (A^G) are determined through Equation (7) [49].

$$A^B = \frac{B_V - B_R}{B_V + B_R} \times 100\%, \quad A^G = \frac{G_V - G_R}{G_V + G_R} \times 100\% \quad (7)$$

The broad-spectrum anisotropy factor (A^U) can be calculated from Equation (8) [50].

$$A^U = \frac{B_V}{B_R} + 5 \frac{G_V}{G_R} - 6 \quad (8)$$

The scalar logarithmic Euclidean anisotropy indicator (A^L) is set up according to Equation (9) [51].

$$A^L = \sqrt{\left[\ln \left(\frac{B_V}{B_R} \right) \right]^2 + 5 \left[\ln \left(\frac{G_V}{G_R} \right) \right]^2} \quad (9)$$

For isotropic materials A^B , A^G , A^U , and A^L are expected to be 0. Deviations from zero indicate a degree of anisotropy. In Figure 7b, the results calculated from A^B and A^G demonstrate that the shear anisotropy factor A^G increases with increasing pressure, while the compressive anisotropy factor A^B remains nearly zero at pressures exceeding 5 GPa. Figure 7c illustrates the variation in the broad-spectrum A^U anisotropy index as well as the

Euclidean logarithmic A^L anisotropy index with pressure. Both A^U and A^L also exhibit an increasing trend with increasing pressure. These findings suggest the shear anisotropy of Mg_2Ni to be more pronounced than compressive anisotropy, and that with increasing pressure its anisotropy increases.

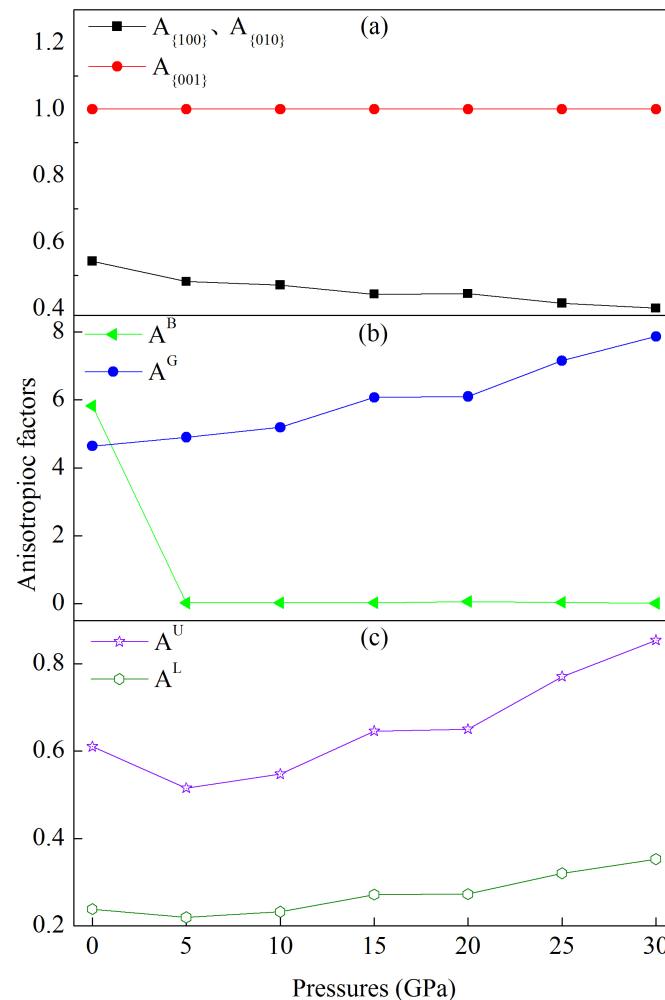


Figure 7. The anisotropy $A_{\{100\}}$, $A_{\{010\}}$, and $A_{\{001\}}$ factors (a), the compressive ratio A^B and the shear ratio A^G (b), as well as broad-spectrum indices A^U and logarithmic Euclidean anisotropy indices A^L (c) are presented for Mg_2Ni at different pressures.

3.4. Speed of Sound at Pressure and Related Properties

Based on the obtained elastic constants C_{ij} , the velocity of pure longitudinal (v_l) and transverse (v_t) sound of hexagonal Mg_2Ni in directions [100] and [001] can be calculated using the method of Brugger [52]. Consequently, the speed of sound in the [100] direction can be calculated as Equation (10) [53,54].

$$[100]v_l = \sqrt{\frac{C_{11} - C_{12}}{2\rho}}, \quad [010]v_{t1} = \sqrt{\frac{C_{11}}{\rho}}, \quad [001]v_{t2} = \sqrt{\frac{C_{44}}{\rho}} \quad (10)$$

The formula for the speed of sound in the [001] is given in Equation (11) [53,54].

$$[001]v_l = \sqrt{\frac{C_{33}}{\rho}}, \quad [100]v_{t1} = [010] \quad v_{t2} = \sqrt{\frac{C_{44}}{\rho}} \quad (11)$$

Among them, v_{t1} and v_{t2} represent corresponding modes one and two, respectively, while ρ denotes the compound's mass density. The determination of the elastic constants for

these sound velocities also reflect the elastic anisotropy of Mg₂Ni. Furthermore, from the obtained bulk modulus B and shear modulus G , the longitudinal velocity of sound (V_L) and the transverse velocity of sound (V_T) for Mg₂Ni can be calculated. The formulae are given in Equation (12) [55].

$$V_L = \sqrt{\frac{3B + 4G}{3\rho}}, \quad V_T = \sqrt{\frac{G}{\rho}} \quad (12)$$

In addition, we can calculate the average sound velocity using Equation (13) [56].

$$V_M = \left[\frac{1}{3} \left(\frac{1}{V_L^3} + \frac{2}{V_T^3} \right) \right]^{-\frac{1}{3}} \quad (13)$$

Figure 8 presents the longitudinal and transverse sound velocity calculations for Mg₂Ni at various pressures. The data clearly illustrate a significant increase in the [100] transverse sound velocity (v_{t1}) of the single crystal as pressure rises. Pressurized to 0–5 GPa, the [001] longitudinal sound velocity (v_l) decreases with increasing pressure, but it increases as the pressure exceeds 5 GPa. Meanwhile, the other sound velocity values show a slight increase with rising pressure. These findings suggest that Mg₂Ni demonstrates sound velocity anisotropy and exhibits an increase in sound velocity with pressure.

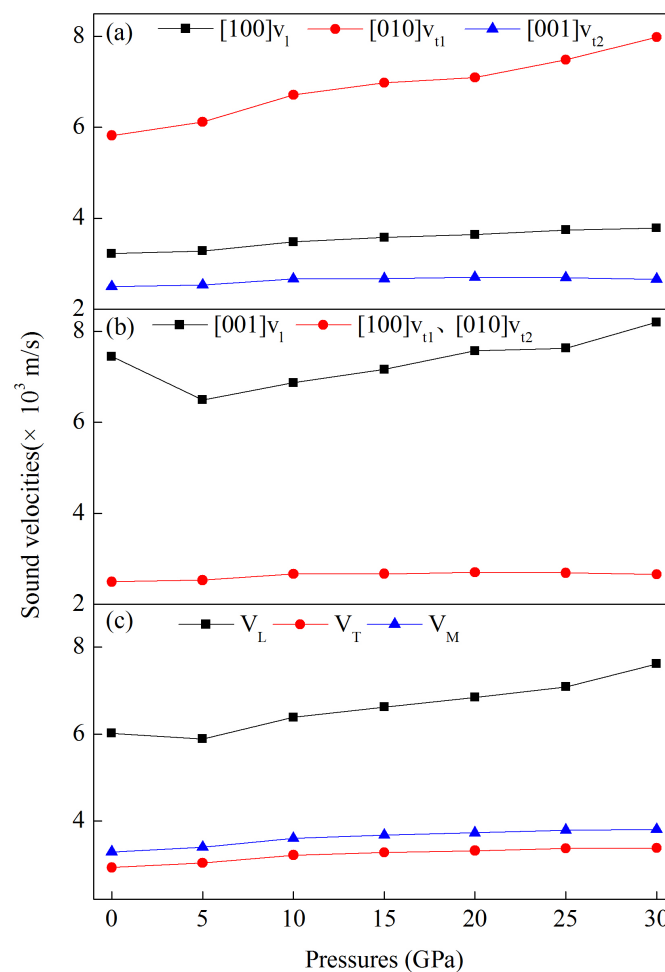


Figure 8. (a) Velocities of longitudinal and transverse sound (v_l , v_{t1} , and v_{t2}) of Mg₂Ni in the [100] direction at different pressures; (b) velocities of longitudinal and transverse sound (v_l , v_{t1} , and v_{t2}) of Mg₂Ni in the [001] direction at different pressures; and (c) longitudinal sound velocity (V_L), transverse sound velocity (V_T) and mean sound velocity (V_M) of Mg₂Ni crystals at different pressures.

Based on the acquired speed of sound data, the temperature in Debye can be calculated using Equation (14) [56].

$$\Theta_D = \frac{h}{k_B} \left[\frac{3n}{4\pi} \left(\frac{N_A \rho}{M} \right) \right]^{\frac{1}{3}} V_M \quad (14)$$

where the parameters h , k_B , n , N_A , and M represent Planck's constant, Boltzmann's constant, the number of atoms in the molecular formula, Avogadro's number, and the molecular weight, respectively.

Figure 9 shows the Debye temperature of Mg_2Ni for different pressures. It is evident from the figure that the Debye temperature of the Mg_2Ni alloy rises with increasing pressure. This phenomenon can be attributed to pressure's influence on the electron structure and interatomic interactions within the material. Under high pressure, the interatomic distance decreases, thereby intensifying interatomic interactions. This heightened interaction subsequently elevates the material's Debye temperature, resulting in heightened thermal stability and resistance to deformation under high pressure. Consequently, the Debye temperature of the Mg_2Ni escalates with increasing pressure.

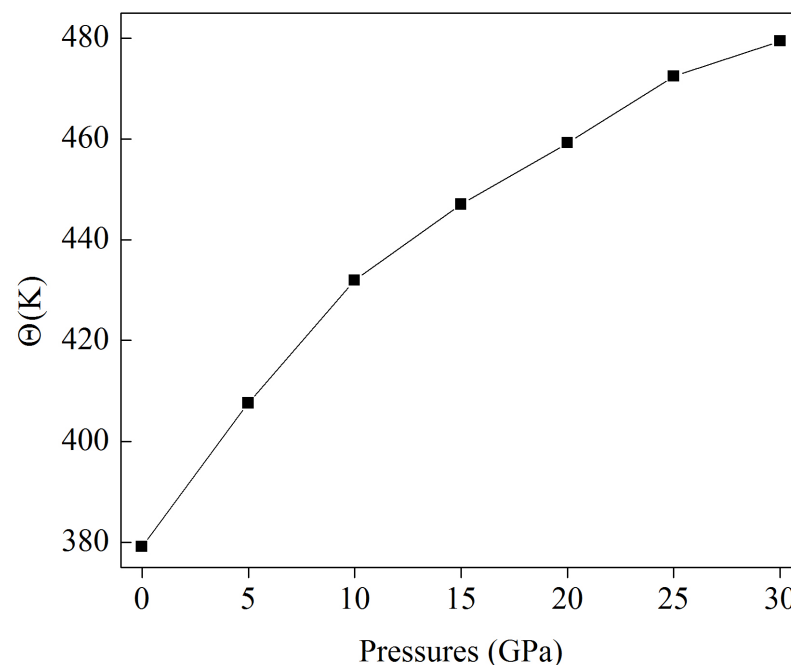


Figure 9. Mg_2Ni alloy's Debye temperature at various pressures.

4. Conclusions

This study comprehensively investigates the mechanical and structural properties of Mg_2Ni materials at different pressures via a first-principles analysis. The findings reveal a decrease in the values of a/a_0 and c/c_0 lattice parameters as pressure increases. Specifically, the values of C_{13} and C_{33} decrease at a hydrostatic pressure of 5 GPa, while the values of C_{11} and C_{13} increase with further increases in pressure beyond 5 GPa. Moreover, all other elastic constants exhibit a monotonic increase from 0 to 30 GPa, with growth rates of C_{11} and C_{12} exceeding those of C_{44} and C_{66} . Pressurized to 0–30 GPa, Mg_2Ni satisfies the mechanical stability criterion, indicating its stable existence within this pressure range. Furthermore, the Poisson's ratio of Mg_2Ni consistently exceeds 0.26 in the pressure range 0–30 GPa, signifying ductility, and demonstrating consistency with the B/G value. The hardness of Mg_2Ni increases in the pressure range 0–5 GPa, but decreases above 5 GPa. Additionally, Mg_2Ni 's shear anisotropy is stronger than its compressive anisotropy, and increases with increasing pressure. Both the sonic anisotropy and the Debye temperature of Mg_2Ni increase with rising pressure. This study serves as a critical reference for gaining deeper understanding of

the Mg₂Ni alloys mechanical properties under different pressure conditions, thus offering valuable insights for its application and property optimization.

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