Pressure-Induced Phase Transition and Mechanical Properties of Mg$_2$Sr Intermetallics

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Abstract: A pressure-induced phase transition of Mg$_2$Sr intermetallics from the low-pressure C14-type phase to an orthorhombic phase (space group Cmcm, $Z = 4$) at a high pressure of 21.0 GPa was firstly predicted using first-principles calculations combined with unbiased swarm structure searching techniques. The phase transition was identified as a first-order nature with a volume drop of 4.7%, driven by the softening of elastic behavior at high pressure. Further phonon calculations indicate that the newly predicted orthorhombic phase is dynamically stable at high pressure and ambient pressure. The mechanical properties including the elastic anisotropy of this orthorhombic phase were thus fully studied at ambient pressure. The elastic anisotropy behavior of this orthorhombic phase was investigated by the distributions of elastic moduli. The evidence of the bonding nature of Mg–Sr was also manifested by density of states (DOS) and electronic localization function (ELF) calculations.

Keywords: intermetallics; phase transition; elastic anisotropy; electronic structure

1. Introduction

The study of Mg intermetallics has been attracting much attention because of their important applications in the automobile and aerospace industries [1,2]. Among the Mg-based intermetallics, the Mg–RE (RE = Ca, Sr, and Ba) system’s intermetallic compounds have emerged as promising candidate materials for transportation, aeronautical, and helicopters [3,4] and have thus generated significant interest over the past few decades. The binary phase diagrams of Mg–Ca, Mg–Sr, and Mg–Ba have been investigated for a long time, and different stable intermetallics have been found in these systems [5–8]. Due to their importance, extensive studies have been undertaken of crystal structures and lattice parameters [9–11], as well as thermodynamic properties [12,13] for these Mg-based intermetallics. In the Mg–Sr system is a typical Laves phase Mg$_2$Sr, the heat formation of which was firstly measured by King and Kleppa [14] by means of tin solution calorimetry. In a recent work, Aljarrah and Medraj [15] reoptimized the Mg–Sr system in the CALPHAD approach considering all the available experimental data on the phase diagram and provided the crystallographic data, heat formation, and lattice parameters of four intermetallic compounds (Mg$_2$Sr, Mg$_{38}$Sr$_9$, Mg$_{23}$Sr$_6$, and Mg$_{17}$Sr$_2$). The heat formation of Mg$_2$Sr reported by Aljarrah and Medraj is in agreement with that of Yang et al. [16], who also investigated the elastic property and density of state (DOS) of this intermetallic phase.

More recently, the mechanical properties, electronic structures, as well as thermodynamic properties of the Mg$_2$Sr Laves phase under high pressure have been systematically investigated using the first-principles calculations by Mao et al. [17]. These extremely important results are...
significant to extend our knowledge to materials performance under extremely severe environments and will inevitably advance our understanding of high-pressure behaviors for other Mg intermetallics. The pressure-induced phase transition sequence of compounds such as Mg$_2$Si has been determined with the aid of experimental and theoretical studies [18]. However, the peculiarity and the absence of further characterized high-pressure phases and related fundamental mechanical properties prompted our endeavor to investigate Mg$_2$Sr intermetallics at a higher pressure. It is well known that high-pressure research leads to the identification of novel behavior of solids and the exploration of potential technological materials, since pressure can significantly alter the electronic bonding state to modify the physical properties, to induce the structural phase transition, or both. In addition, from the recent work for Mg$_2$Sr [17], its elastic parameters exhibit a clear softening trend at an elevated pressure, especially for single crystal elastic constant $C_{44}$, signifying its structural instability at high pressures. Therefore, we here performed extensive structure searches to explore the crystal structures of Mg$_2$Sr over a range of pressures (0–50 GPa), based on a global minimization of free-energy surfaces merging ab initio total energy calculations via the particle swarm optimization technique [19]. Indeed, the pressure-induced transition into an orthorhombic phase ($C_{mcm}$, $Z = 4$) for Mg$_2$Sr at 21.0 GPa was firstly predicted. First-principles calculations were then performed to investigate the crystal structures, mechanical, and electronic properties for this novel orthorhombic phase.

2. Computational Methods

The high-pressure structure searches of Mg$_2$Sr were performed by the recently developed Crystal structure AnaLYsis by Particle Swarm Optimization (CALYPSO) package [19,20], which has perfectly predicted the crystal structures of a diverse variety of materials [21–25]. In more detail, the variable-cell structure predictions were executed at 0, 10, 25, and 50 GPa with systems containing 1–6 formula units (f.u.) in the simulation cell. Structural relaxation, total energy, and electronic structure calculations were mainly performed using the density functional theory with the Perdew–Burke–Ernzerhof generalized gradient approximation [26,27], as implemented in the VASP code [28]. The projector augmented wave (PAW) method [29] was used to describe the electron-ion interactions, with $3s^2$ and $4s^24p^65s^2$ treated as valence electrons for Mg and Sr, respectively. A kinetic energy cutoff of 400 eV for the plane-wave expansion and dense $k$-point with grid density of $2\pi \times 0.03$ Å$^{-1}$ (Monkhorst–Pack scheme) [30] were used in the Brillouin zone integration. The enthalpy and electronic band structure were calculated using the tetrahedron method with Blöchl corrections. Finite displacement method [31], which is based on first-principles calculations of total energy, Hellman–Feynman forces, and the dynamical matrix as implemented in the PHONOPY package to calculate the phonon spectra. The supercell of $3 \times 3 \times 3$ original cell containing 162 atoms was adopted in the phonon calculations for Mg$_2$Sr. The strain-stress method was applied to calculate the single crystal elastic constants, and the polycrystalline bulk modulus and shear modulus were thus derived from the Voigt–Reuss–Hill averaging scheme [32].

3. Results and Discussion

Using the CALYPSO package, at pressures of 0 and 10 GPa, the experimental C14-type phase of Mg$_2$Sr with space group $P6_3/mmc$ ($Z = 4$, see Figure 1a) was successfully reproduced from a global structure search, validating our method adopted here. In Figure 1a, the C14-type phase contains twelve atoms per unit cell with eight Mg atoms occupying the $2a$ and $6h$ positions and four Sr atoms occupying the $4f$ positions. At ambient pressure, the optimized equilibrium structural parameters for C14-type phase are $a = 6.456$ Å, $c = 10.45$ Å, and $V_0 = 377.236$ Å$^3$, which are all in good agreement with the available experimental data ($a = 6.484$ Å, $c = 10.451$ Å, and $V_0 = 380.5$ Å$^3$) [33] and theoretical values [17]. In addition, the theoretical equations of states (EOS) of Mg$_2$Sr studied here were determined by fitting the total energies as a function of the volumes based on the Birch–Murnaghan EOS. The obtained bulk modulus $B_0$ and its pressure derivative $B_0\prime$ of Mg$_2$Sr (25.946 GPa and 3.644) also agree well with the previous theoretical values [17]. The success in the prediction of experimental C14-type phase gives us confidence to further explore the high-pressure phases of Mg$_2$Sr. For higher pressures at 25 and 50 GPa,
a novel orthorhombic phase with \textit{Cmcm} space group (\(Z = 4\), hereafter denoted as HP; see Figure 1b) was discovered for Mg\(_2\)Sr as the most energetically stable. At 30 GPa, the optimized lattice parameters of HP-Mg\(_2\)Sr are \(a = 8.585\) Å, \(b = 5.399\) Å, and \(c = 4.754\) Å, with Mg and Sr atom occupying the 8\(g\) (0.329, 0.366, 0.25) and 4\(c\) (0, 0.346, 0.25) positions, respectively. The projection of the orthorhombic HP phase on the \(ac\)-plane is presented in Figure 1c, from which the HP phase possesses alternative stacking of double Mg and single Sr layers along the \(a\)-direction. Each Mg ion is coordinated with five Sr ions, and each Sr ion is coordinated with ten Mg ions. Physically, the phonon is a strict measure for structural dynamic stability. We thus carefully checked the phonon frequency curves of HP-Mg\(_2\)Sr at 50 GPa (Figure 2a) and 0 GPa (Figure 2b). In Figure 2, there is no imaginary phonon frequency in the entire Brillouin zone, i.e., the HP-Mg\(_2\)Sr is dynamically stable at high and ambient pressures. The lower frequencies of the phonon density of states are dominated by lattice dynamics of heavy Sr atoms and higher frequencies by light Mg atoms.

Figure 1. Crystal structures of Mg\(_2\)Sr. (a) Low-pressure C14-type phase; (b) The predicted high-pressure orthorhombic \textit{Cmcm} phase; (c) The projection of orthorhombic \textit{Cmcm} phase on \(ac\)-plane. The large and small balls denote Sr and Mg atoms, respectively.

Figure 2. Phonon curves of the orthorhombic \textit{Cmcm} phase at (a) 50 GPa and (b) 0 GPa.

To determine the phase transition pressure point of Mg\(_2\)Sr, the enthalpy differences curves of the predicted HP phase relative to the C14-type phase are presented in Figure 3a. We optimized these two structures at many more pressure points up to 50 GPa with certain pressure intervals. Figure 3a confirms that the predicted HP phase becomes more stable than the experimental C14-type phase above 21.0 GPa, where the current experimental techniques are readily accessible. Meanwhile, as shown in Figure 3b, one can see that the C14-type \(\rightarrow\) HP phase transition is first-order with a clear volume contraction of 4.7%. Such an obvious volume reduction at the transition is easy to detect in a high
pressure X-ray powder diffraction experiment. The pressure dependence of lattice constants for two phases are also plotted in Figure 3c to complement further experiments. The pressure dependence of elastic constants is a very important indicator of the mechanical stability of crystal. We first calculated the single crystal elastic constants of C14-type phase at ambient pressure, as tabulated in Table 1 together with the theoretical results for comparisons. From Table 1, one can see that the calculated elastic moduli of HP and C14-type phases are lower than those experimental data of pure Mg2Sr. These results suggest that the C14-type phase is mechanically unstable when \( P > 26.6 \) GPa under high pressure. We thus conclude that there must be a structural phase transition occurring in the pressures according to relations of the mechanical stability under isotropic pressure, as suggested by Karki et al. [35] and Wang et al. [36]. These behaviors further confirmed the accuracy of the predicted phase transition pressure of Mg2Sr, although the obtained transition pressure (26.6 GPa) is relative larger than that (21.0 GPa) obtained from the enthalpy differences curves of Figure 3a.

![Figure 3.](image)

**Figure 3.** (a) Enthalpy differences of high-pressure Cmcm phase relative to the low-pressure P63/mmc phase as a function of pressure; (b) The calculated volumes as a function of pressure for the P63/mmc and Cmcm phases; (c) The calculated lattice parameters as a function of pressure for the P63/mmc and Cmcm phases; (d) The calculated \( \tilde{C}_{44}, \tilde{C}_{11} - |\tilde{C}_{12}| \) and \( \tilde{C}_{33}(\tilde{C}_{11} + \tilde{C}_{12}) - 2\tilde{C}_{13}^2 \) under different isotropic pressures.

**Table 1.** Calculated elastic constants \( C_{ij} \) (GPa), bulk modulus \( B \) (GPa), shear modulus \( G \) (GPa), Young’s modulus \( E \) (GPa), and Poisson’s ratio \( \nu \) for Mg2Sr.

| Mg2Sr  | Source | \( C_{11} \) | \( C_{22} \) | \( C_{33} \) | \( C_{44} \) | \( C_{55} \) | \( C_{66} \) | \( C_{12} \) | \( C_{13} \) | \( C_{23} \) | \( B \) | \( G \) | \( E \) | \( \nu \) |
|--------|--------|--------------|--------------|--------------|-------------|-------------|-------------|-------------|-------------|-------------|---------|---------|---------|-------|
| C14-type | Present | 49.9 | - | 56.9 | 14.2 | - | - | 17.4 | 10.2 | - | 25.8 | 16.6 | 41.0 | 0.235 |
| Theory | a | 43.8 | - | 57.2 | 12.4 | - | - | 19.8 | 10.6 | - | 25.2 | 13.8 | 36.1 | 0.360 |
| Theory | b | 43.7 | - | 56.5 | 12.4 | - | - | 20.1 | 11.9 | - | 25.4 | 13.7 | 34.8 | 0.230 |
| HP | Present | 43.1 | 42.9 | 52.0 | 17.6 | 13.2 | 13.7 | 15.7 | 12.6 | 10.7 | 24.0 | 15.3 | 37.9 | 0.237 |

\( ^a \) Ref. [34]; \( ^b \) Ref. [17].
Compared with the experimental C14-type phase, using the same method mentioned above, the mechanical properties (including the elastic stability, incompressibility, rigidity, and elastic anisotropy) of this predicted HP phase were fully studied at ambient pressure. The resulting single crystal elastic constants and the derived Hill elastic moduli are listed in Table 1. The mechanical stability of the HP phase satisfies the Born–Huang criterion for an orthorhombic crystal [C_{11} > 0, C_{44} > 0, C_{55} < 0, C_{66} < 0, C_{11}C_{22} > C_{12}^2, C_{11}C_{22}C_{33} + 2C_{12}C_{13}C_{23} − C_{11}C_{23}^2 − C_{22}C_{13}^2 − C_{33}C_{12}^2 > 0] [37], thus confirming that this HP phase is mechanically stable at ambient conditions. Moreover, the obtained elastic constants possess the trend of C_{11} ≈ C_{22} < C_{33}, indicating that the bonding between nearest neighbors along the [001] planes is stronger than those along the [100] and [010] planes. Both the calculated elastic moduli of HP and C14-type phases are lower than those experimental data of pure Mg metal (\(B = 36.9\) GPa, \(E = 19.4\) GPa, and \(\mu = 49.5\) GPa) [38]. Traditionally, and for ease of manipulation, the elastic properties of an anisotropic material were replaced by those of an “equivalent” isotropic material. Essentially, all the known crystals are elastically anisotropic, and the anisotropy of elasticity is an important implication in engineering science and crystal physics, such as microcracks, anisotropic plastic deformation, and elastic durability. To intuitively illustrate the elastic anisotropy of this predicted orthorhombic phase, the directional dependence of elastic moduli were systematically investigated. The calculations of elastic moduli crystal orientation dependence conducted here are similar to our previous studies [39]. Executing the appropriate coordinate system transformations for the compliances allows for the directional dependence of elastic moduli to be systematically investigated. The calculations of elastic moduli crystal orientation dependence conducted here are similar to our previous studies [39].

From Figure 4a,c, one can see that this HP phase exhibits a weak elastic anisotropy, for its bulk modulus and Young’s modulus distributions with the nonspherical nature. Compared with the experimental C14-type phase, using the same method mentioned above, the mechanical properties (including the elastic stability, incompressibility, rigidity, and elastic anisotropy) of this predicted HP phase were fully studied at ambient pressure. The resulting single crystal elastic constants and the derived Hill elastic moduli are listed in Table 1. The mechanical stability of the HP phase satisfies the Born–Huang criterion for an orthorhombic crystal [C_{11} > 0, C_{44} > 0, C_{55} < 0, C_{66} < 0, C_{11}C_{22} > C_{12}^2, C_{11}C_{22}C_{33} + 2C_{12}C_{13}C_{23} − C_{11}C_{23}^2 − C_{22}C_{13}^2 − C_{33}C_{12}^2 > 0] [37], thus confirming that this HP phase is mechanically stable at ambient conditions. Moreover, the obtained elastic constants possess the trend of C_{11} ≈ C_{22} < C_{33}, indicating that the bonding between nearest neighbors along the [001] planes is stronger than those along the [100] and [010] planes. Both the calculated elastic moduli of HP and C14-type phases are lower than those experimental data of pure Mg metal (\(B = 36.9\) GPa, \(E = 19.4\) GPa, and \(\mu = 49.5\) GPa) [38]. Traditionally, and for ease of manipulation, the elastic properties of an anisotropic material were replaced by those of an “equivalent” isotropic material. Essentially, all the known crystals are elastically anisotropic, and the anisotropy of elasticity is an important implication in engineering science and crystal physics, such as microcracks, anisotropic plastic deformation, and elastic durability. To intuitively illustrate the elastic anisotropy of this predicted orthorhombic phase, the directional dependence of elastic moduli were systematically investigated. The calculations of elastic moduli crystal orientation dependence conducted here are similar to our previous studies [39]. Executing the appropriate coordinate system transformations for the compliances allows for the directional dependence of elastic moduli to be systematically investigated. The calculations of elastic moduli crystal orientation dependence conducted here are similar to our previous studies [39].

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accords well with the smallest anisotropy within ab planes (see Figure 4d). Similarly, the orientation dependence of the shear modulus on the stress directions within the four main crystal planes were also conducted, as plotted in Figure 5b. For the (100) shear plane with the shear stress direction rotated from [100] to [010], the direction cosines are α1 = cos θ, β1 = sin θ, γ1 = 0, α2 = β2 = 0, and γ2 = 1, where θ is the angle between the [100] and shear stress direction. From Equation (3), one can deduce the shear modulus expressed as
\[ G_{12}^{−1} = s^{55} + (s^{44} − s^{55}) \sin^2 \theta. \]
For HP-Mg2Sr, \( s^{44} < s^{55} \), the shear modulus is the largest along [010] and is the smallest along [001]. Among these four main crystal planes, it should be noted that the shear moduli within the (100) shear plane are the smallest with its minimum \( G_{(100)}[001] = 13.2 \) GPa and maximum \( G_{(100)}[010] = 13.7 \) GPa values, and are almost independent of any shear directions. Thus, the (100) shear plane may be viewed as the cleavage plane of HP-Mg2Sr.
4. Conclusions

To conclude, the pressure-induced phase transition of Mg$_2$Sr was predicted using a particle swarm optimization algorithm in crystal structure prediction. An orthorhombic high-pressure phase (space group Cmcm, Z = 4) of Mg$_2$Sr was uncovered at 21.0 GPa. The transition of low-pressure
C14-type phase to this orthorhombic HP phase was characterized as a first-order nature, driven by the softening of elastic behavior at high pressure. The elastic anisotropy of the predicted orthorhombic phase was demonstrated by the orientational distributions of the elastic moduli. The shear modulus is found to be the smallest within the (100) crystal plane, which may be viewed as its cleavage plane. Detailed analyses of the DOS and ELF reveal that the chemical bonding in the orthorhombic phase is a complex mixture of covalent and ionic characters.

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