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Emine KALE AYDIN[a*]
Emel KILIT DOGAN[b]
Sinem ERDEN GULEBAGLAN[c]

[a] Lec., Van Yuzuncu Yil University, eminekaleaydin@yyu.edu.tr
[b] Prof., Van Yuzuncu Yil University, ekilit@yyu.edu.tr
[c] Prof., Van Yuzuncu Yil University, sinemerden@gmail.com

* Corresponding Author

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Analysis of Electronic, Dynamic and Elastic Properties of The Half-Heusler MgScB Crystal Using Density Functional Theory

Abstract

The electronic, dynamic, and elastic properties of the MgScB half-Heusler crystal are investigated using density functional theory (DFT) calculations as executed in the Quantum Espresso computational suite. An analysis was performed on a cubic MgScB half-Heusler crystal using the generalized gradient approach (GGA). According to the results obtained, the band gap of 0.16 eV was found for the half-Heusler MgScB crystal, and based on this finding, it was concluded that the MgScB crystal exhibited semiconductor properties. The dynamic properties were also predicted using linear response density functional perturbation theory. The half-Heusler MgScB crystal exhibits dynamically stable behavior. To determine the elastic properties of the half-Heusler MgScB crystal, the elastic stiffness constants and some important elastic constants were calculated. It was concluded that the crystal showed brittle properties.

Keywords: DFT, Half-Heusler, MgScB, Semiconductor

Yoğunluk Fonksiyonel Teorisi Kullanılarak Yarı Heusler MgScB Kristalinin Elektronik, Dinamik ve Elastik Özelliklerinin Analizi

Öz

MgScB yarı-Heusler kristalinin elektronik, dinamik ve elastik özellikleri, Quantum Espresso hesaplama paketinde gerçekleştirilen yoğunluk fonksiyonel teorisi (DFT) hesaplamaları kullanılarak incelenmiştir. Genelleştirilmiş gradyan yaklaşımı (GGA) kullanılarak kübik MgScB yarı-Heusler kristali üzerinde bir analiz gerçekleştirilmiştir. Elde edilen sonuçlara göre, yarı-Heusler MgScB kristali için 0,16 eV'lik bir enerji bandı farkı bulunmuştur; bu sonuca göre, MgScB kristalinin yarı iletken özellikler sergilediği sonucuna varılmıştır. Dinamik özellikler de doğrusal tepki yoğunluk fonksiyonel pertürbasyon teorisi kullanılarak öngörülmüştür. Yarı-Heusler MgScB kristali dinamik olarak kararlı bir davranış sergilemektedir. Yarı-Heusler MgScB kristalinin elastik özelliklerini belirlemek için elastik sertlik sabitleri ve bazı önemli elastik sabitler hesaplanmıştır. Kristalin kırılgan özellikler sergilediği sonucuna varılmıştır.

Anahtar kelimeler: DFT, Half-Heusler, MgScB, Yarı iletken

1.Introduction

The general formula of half-Heusler crystals is ABC. In general, the C element is expressed as the main group element, and A and B elements are expressed as transition metals in the formation of these structures. The half-Heusler crystals have a cubic structure with the ($F\bar{4}3m$) space group [1, 2]. Half-Heusler crystals

are highly functional materials. Since these materials exhibit both ferromagnetic and antiferromagnetic properties due to interatomic interactions, they are considered an important research area for experimental or theoretical studies. Half-Heusler crystals are suitable materials for magnetic memory devices and spintronic applications [3,4]. Magnetic Heusler crystals are gaining importance due to the spin Hall effect [5,6].

Half-Heusler crystals, in addition to their magnetic properties, also exhibit significant potential for thermoelectric applications. Such materials enable the conversion of heat into electricity owing to their tunable electronic structures and favorable phonon transport properties [7]. Furthermore, their semiconducting behavior and adjustable band gaps make Half-Heusler crystals highly suitable candidates for optoelectronic and electronic devices [8]. These materials demonstrate efficiency in various aspects of advanced technological applications. In this context, the MgScB half-Heusler crystal is important for future device technologies as a multifunctional material possessing magnetic, electronic, and thermoelectric properties. Considering the potential of the MgScB half-Heusler crystal in thermoelectric and optoelectronic applications, it is important to investigate its physical properties theoretically.

Ahmed et al. conducted a study on the thermal conductivity and the electronic properties of LiMgN, NaMgN and KMgN half-Heusler crystals [9]. Abada and Marbouh calculated the structural, magnetic, electronic and elastic properties of d^0 half-metallic half-Heusler MgCaB crystal by using density functional theory [10]. Sun et al. investigated the electronic, transport and thermal conductivity properties of BCaGa, BMgGa and BBeGa half-Heusler materials and made comparisons [11]. Islam et al. calculated the magnetic and spin Hall conductivity properties of MgMnGe half-Heusler crystals by using DFT [12]. Umamaheswari et al. investigated the structural, electronic and magnetic properties of LiMgB, NaMgB, KMgB and RbMgB half-Heusler crystals using DFT [13]. Mehnane et al. determined the structural, electronic and optical properties of 36 crystals, including KMgN, KMgP, KMgAs, LiMgN, LiMgP, LiMgAs, NaMgN, NaMgP and NaMgAs half-Heusler crystals [14]. Al-zyadi et al. studied the electronic and magnetic properties of the MgCaB half-Heusler crystal, which is a suitable material for spintronic applications [15]. Ahmad and Mehmood predicted the structural, elastic, mechanical, electronic, magnetic and optical properties of CrScP, CrScAs and CrScSb half-Heusler compounds using the WIEN2k package [16].

The present study investigates the structural, electronic, elastic and dynamic properties of the MgScB half-Heusler crystal. When the studies carried out so far were examined, it was found that there was only one study on the MgScB half-Heusler crystal, by T. Gruhn [17]. The motivation for the study was to reveal properties of the MgScB crystal, which had not been determined before, given the importance of the half-Heusler crystal family in applications. We believe the results we obtained will be a starting point for further theoretical and experimental studies.

2. Material and Method

The properties of the MgScB half-Heusler crystal were investigated using the Quantum ESPRESSO [18] package program, which is based on density functional theory. The exchange-correlation energy of the electrons was described using the Generalized Gradient Approximation developed by Perdew, Burke and Ernzerhof [19]. The pseudopotentials used in the calculations for elements Mg, Sc, and B are of the Perdew-Burke-Ernzerhof (PBE) function type, generated using the Martins-Troullier method. Same types of pseudopotentials were used in all calculations. From here, the Kohn-Sham equations were solved [20]. The ground state density and energy are determined by solving the Kohn-Sham equations using the Self-Consistent Field (SCF) method. In Non-Self-Consistent Field (NSCF) calculations, electronic properties are determined with a small number of k-points using the constant electron density found in the SCF calculations. To determine the optimal cut-off value, ground-state energies were calculated across a range of energy levels. The results obtained are given in Table 1. Based on this data, the cut-off energy for the plane-wave basis set was selected as 80 Ry.

Table 1. The ground state energy dependence on cut-off energy (E_{cut}) for the MgScB half- Heusler crystal.

E cut (Ry)	E (eV)
30	-13.12725
40	-13.14813
50	-13.14821
60	-13.14909
70	-13.14922
80	-13.14930
90	-13.14933
100	-13.14935

Next, the ground state energy values corresponding to the various k-point values were calculated. The results obtained are given in Table 2. According to the results shown in Figure 1, for self-consistent calculations, the Brillouin zone k-grid was used as 12x12x12 [21]. In our calculations, we recalculated the electron density and energy at each step, choosing an energy difference of 1.0 x 10^{-8} Ry between successive steps. The states of Mg ($3s^2$), Sc ($4s^2 3d^1$), and B ($2s^2 2p^1$) were selected as valence electrons.

Table 2. The ground-state energy dependence on k-point for the MgScB half- Heusler crystal.

k-point	E (eV)
4	-13.1469
5	-13.1481
6	-13.1487
7	-13.1490
8	-13.1491
9	-13.1492
10	-13.1492
11	-13.1492
12	-13.1492
13	-13.1492
14	-13.1493
15	-13.1493
16	-13.1493

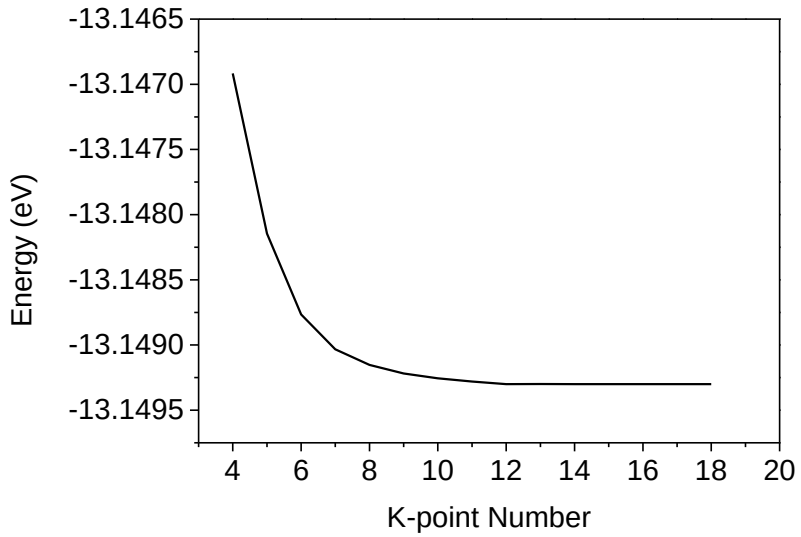

Figure1. The ground-state energy dependence on k-point for the MgScB half-Heusler crystal. Energy values are given in

eV units.

Density Functional Perturbation Theory determines the response of crystal structures to atomic displacements or small perturbations such as electric or magnetic fields. Using this method, the energy derivatives of a crystal with a known ground state can be calculated to determine its dynamic properties. For this reason, the dynamic properties of the MgScB half-Heusler crystal are calculated by the Density Functional Perturbation Theory [22]. In phonon calculations, q vectors represent the wave vector of a vibration mode. In our calculations, a 4x4x4 q-point grid is chosen to account for phase differences between unit cells and for short-wavelength vibrations. The dynamic matrices in the calculations are obtained using a 4x4x4 q-point Brillouin zone grid. The spin-orbit interaction is neglected in all investigated properties of the MgScB half-Heusler crystal. Spin-orbit interaction is important in heavy elements (especially 4d and 5f). If spin-orbit interaction is not considered in heavy-element systems, errors in the energy band gap may occur. However, since the elements forming the crystal under investigation are not heavy, it is noticed that this will not cause very large changes in the calculated energy band value. The calculation of elastic constants was performed using the strain–stress method within the framework of Density Functional Theory (DFT). In this method, elastic constants are primarily derived by calculating the total energy or the stress tensor using small strains.

3. Results

In this study, the cubic MgScB half-Heusler crystal is analyzed using the GGA approach, and its structural properties are first determined. Subsequently, the electronic, dynamic, and elastic properties are examined using the calculated values.

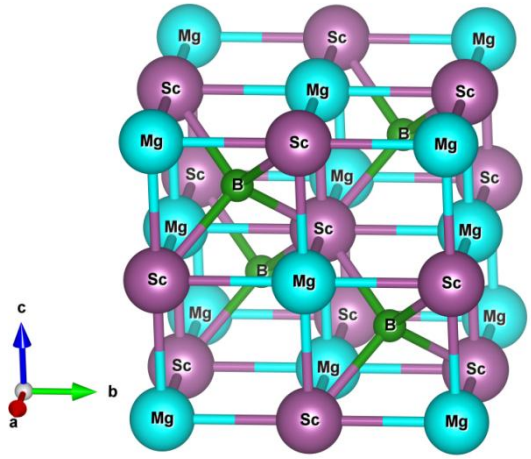

Figure 2. FCC structure of MgScB crystal drawn by Vesta Programme [23]

The cubic MgScB half-Heusler crystal is in space group 216 ($F\bar{4}3m$)and point group $\bar{4}3m$. The unit cell structure of MgScB was modelled using the Vesta program and is displayed in Figure 2. Furthermore, the bonds and bond lengths between Mg-Sc and Sc-B formed in the crystal were calculated with the Vesta program and are given in Table 3.

Table3. Bonds and bond lengths of MgScB

Bonds	Bond lengths(Å)
Mg-Sc	2.9072
Sc-B	4.8207

To study the structural properties of a crystal, various optimizations are required. For this purpose, firstly, the cut-off energy of the MgScB half-Heusler crystal was determined to be 80 Ry by cut-off energy optimization. Subsequently, the number of k points and Monkhorst-Pack partition were calculated by k-point optimization. The Monkhorst-Pack Partition value was determined as 12x12x12. Finally, volume optimization was performed. With this optimization, the lattice parameters and the steady-state volume value of the cubic MgScB half-Heusler crystal were found. The total energy of the crystal at steady-state, also known as ground state energy, is calculated at this stage. In this study, the lattice parameter of MgScB was calculated as 11.0300 Bohr. This value is found to be highly compatible with the literature value of 10.9869 Bohr [17], as reported in the extant literature.

The electronic properties of the cubic MgScB half-Heusler crystal were determined using the lattice parameters calculated in the equilibrium state. The electronic properties of the crystal were calculated and plotted with the Quantum Espresso program. The electronic band structure graph calculated under the GGA approach is shown in Figure 3. Calculations were executed along the $\Gamma - X - W - L - \Gamma - K - W - U$ high symmetry points in the first Brillouin zone and subsequently transferred to the graph. The Fermi energy level is designated as 0 eV on the graph.

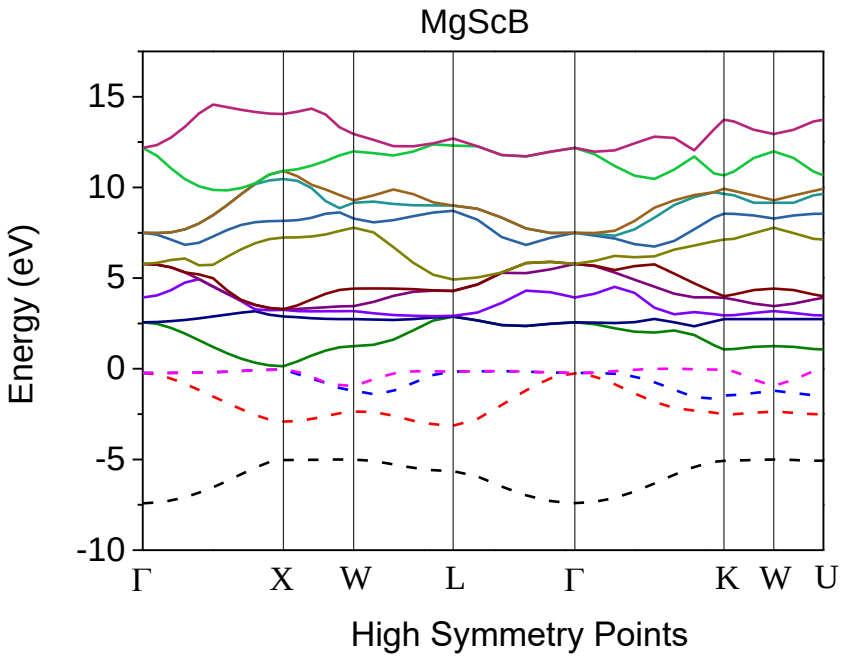

Figure3. Electronic band structure of MgScB crystal calculated by Density Functional Theory under Generalized Gradient Approximation (GGA). Energy values are given in eV units.

As illustrated in Figure 3, the band gap for the MgScB crystal is clear when the 0 eV–2.5 eV region of the energy axis is examined. It has been established that the maximum of the valence band and the minimum of the conduction band are located at the X-symmetry point. The observation that the maximum of the valence band and the minimum of the conduction band coincide at a specific point of symmetry indicates that the MgScB crystal exhibits a direct band gap transition. The conduction band minimum and the valence band maximum at the X symmetry point are separated by 0.16 eV. This value corresponds to the band gap, which is indicative of the semiconductor nature of the MgScB half-Heusler crystal. Moreover, in density functional theory, the Perdew-Burke-Ernzerhof functional can accurately predict bond length and lattice parameters. However, due to the limitations in describing the Van der Waals interaction, the energy band gap may be underestimated. Therefore, results lower than the experimental value may be obtained. Since the d and f orbitals are absent in the crystal structure we are investigating, it is noticed that there will not be significant changes in the obtained results.

The Generalized Gradient Approximation is an approximation that generally incorporates the spatial variation. It is an approximation that yields better results in systems with low energies and large lattice constants. According to the study that revealed the properties of the MgScGa [24] compound, which has a similar structure to the MgScB crystal, it was shown to have a relatively narrow energy band gap. The MgScB crystal, whose properties were also investigated, has a very narrow energy band gap.

The assessment of the density of states is also crucial for further evaluation of the electronic properties after the band structure analysis. The density of states (DOS) is defined as the number of states that occur per unit energy interval. The total and partial density of states (PDOS) for the MgScB crystal were calculated under the GGA approximation. The density of states is expressed in arbitrary units (a.u.), and the energy is measured in electronvolts (eV). As illustrated in Figure 4, the plots of the total density of states of the MgScB crystal and the partial densities of states of the constituent atoms. The contributions of the s, p, d, and f levels of each atom are represented in the graphs by different colors. Density of states plots provide information about the electrical conductivity of a crystal, like the electronic band structure graphs. It represents the conducting, semiconducting, or insulating nature of the crystal.

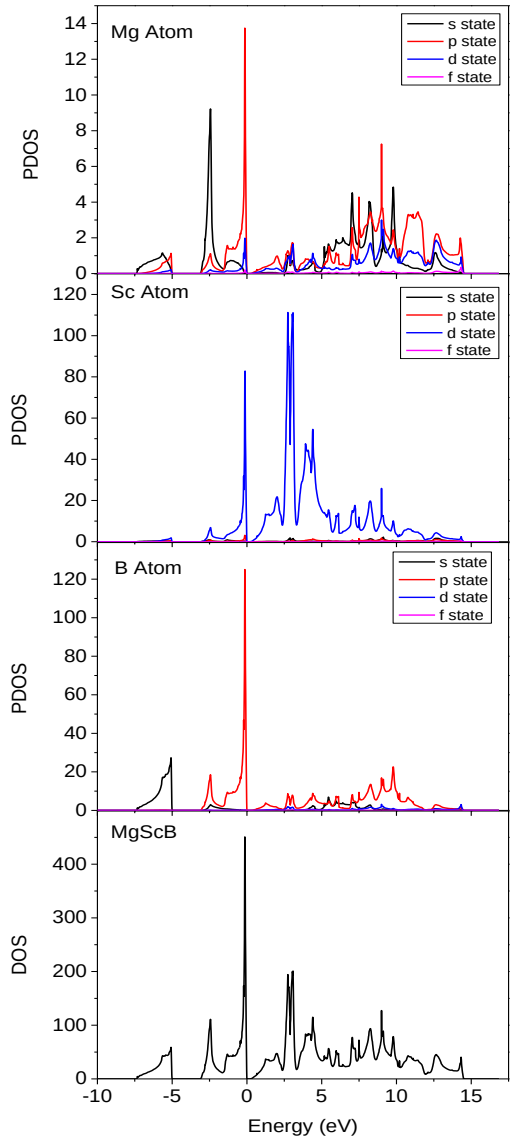

Figure 4. Partial (PDOS) and total density of states (DOS) graphs of MgScB crystal calculated by Density Functional Theory under Generalized Gradient Approximation (GGA). DOS and PDOS are given in arbitrary units (a.u.), and energy values are given in eV units.

Looking at the graph in Figure 4, we can see that the core electrons in the crystal contribute a small portion, whilst the valence electrons provide the dominant contribution to the total density of states. Conduction band electrons also contribute significantly to the total density of states. From the partial density of states plots shown in Figure 4, it can be seen which electron energy levels of each atom in the crystal contribute to the density of states. A thorough examination of the graphs in Figure 4 reveals that the electrons at the s level of the magnesium (Mg) atom contribute slightly to the valence band. In contrast, the electrons at the s and p levels contribute significantly to the valence band, while those at the s, p, and d levels contribute to the conduction band, albeit to a lesser extent. Upon analysis of the partial density of states of the scandium (Sc) atom, it is evident that the electrons at the d level contribute to both the valence and conduction bands at high rates. The electrons at the s level of the boron (B) atom contribute to the lower valence band, while the electrons at the p level contribute to the valence band. However, the contribution to the conduction band is less significant. It has been observed that the electronic band structure and density of state graphs depicted in Figures 2 and 3,

which are instrumental in determining the electronic properties, exhibit compatibility with each other.

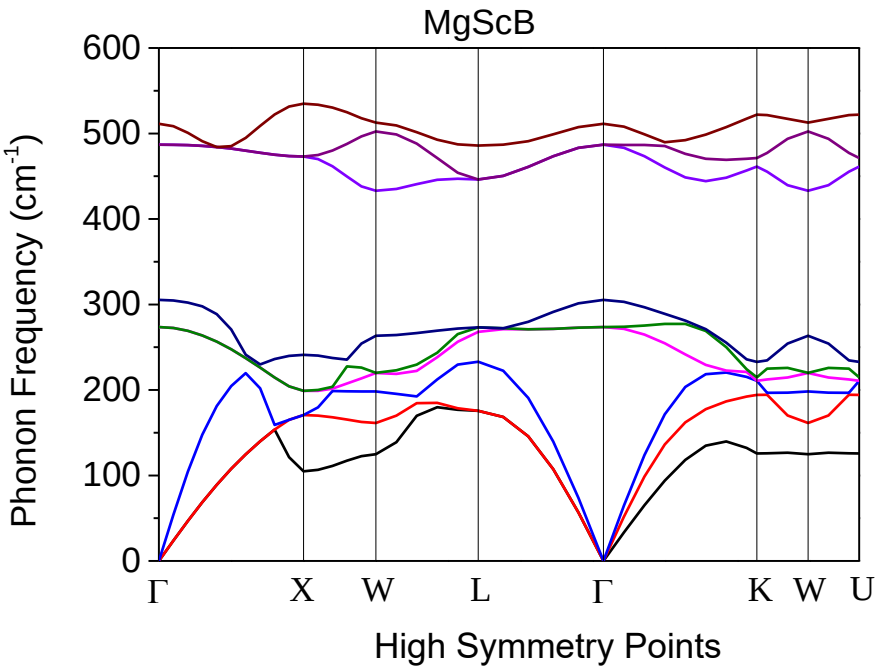

Figure 5. Phonon dispersion curve of MgScB crystal calculated by Density Functional Theory under Generalized Gradient Approximation (GGA). Phonon Frequency values are given in cm^{-1} units.

The dynamic properties were investigated by obtaining the phonon dispersion curve of the MgScB crystal. Since MgScB has 3 atoms in its unit cell, nine dynamical modes occur. The number of dynamic modes is obtained by multiplying the number of atoms by the number of vibration directions (i.e., 3x3=9). As illustrated in Figure 5, the phonon frequencies of these nine dynamical modes are compared with those of the high symmetry modes. The three dynamical modes with the lowest frequencies are acoustic modes. Those have 0 cm^{-1} frequency value for the Γ high symmetry point. The remaining six modes are optical modes. The first three optical modes are found around 300 cm^{-1}, and the second three optical modes are found around 500 cm^{-1}.

Acoustic and optical modes consist of transverse and longitudinal branches. Of the three acoustic modes, the two low-frequency modes are transverse acoustic (TA) modes, and the high-frequency one is a longitudinal acoustic (LA) mode. For the optical modes that appear at 300 cm^{-1}, the two modes with lower frequency are transverse optic (TO) modes, and the one with higher frequency is the longitudinal optical (LO) mode. Also, for the optical modes that appear at 500 cm^{-1}, there are two TO and one LO modes.

The phonon dispersion curves also illustrate the dynamical stability of the material. The material is considered dynamically stable if the acoustic mode frequencies are positive; accordingly, the MgScB crystal exhibits dynamical stability as all its phonon frequencies are positive (Figure 5)

A factor group analysis of the phonon modes of the MgScB half-Heusler crystal was performed using the execution of the Bilbao crystallographic server [25]. This execution is based on group theory. The decomposition of the total representation of Γwas obtained. The irreducible representation of Γ can be written as follows:

$$\Gamma = \Gamma_{Acoustic} + \Gamma_{Optical} \quad (1)$$

The symmetries of this space group are A_1, A_2, E, T_1 and T_2 . However, only T_2 is observed. The acoustic component of Γ is equal to T_2 $(\Gamma_{Acoustic} = T_2)$, and the optical component of Γ is equal to $2T_2(\Gamma_{Optical} = 2T_2)$. Total value of Γ is equal to $3T_2$.

Table 4. Some elastic properties of the MgScB crystal.

Elastic Properties		**Value**
Elastic Stiffness Constants (GPa)	$C_{11} = C_{22} = C_{33}$	200.37
	$C_{44} = C_{55} = C_{66}$	33.61
	$C_{12} = C_{21} = C_{13} = C_{31} = C_{23} = C_{32}$	13.77
Reuss Bulk Modulus, B_R (GPa)		75.97
Voigt Bulk Modulus, B_V (GPa)		75.97
Hill Bulk Modulus, B_{VRH} (GPa)		75.97
Reuss Shear Modulus, G_R(GPa)		45.17
Voigt Shear Modulus, G_V(GPa)		57.49
Hill Shear Modulus, G_{VRH}(GPa)		51.33
Young Modulus, E (GPa)		125.68
Poisson Ratio, ν (-)		0.22
Pugh's Ratio, k=B_{VRH}/G_{VRH} (-)		1.48
Debye Temperature, Θ_D (K)		123.84

The elastic properties of the MgScB crystal are also investigated within this study. To reveal the elastic properties, the elastic stiffness constants were first computed. Elastic stiffness constants are the ratio between the stress and the strain. Since MgScB is a cubic crystal, the number of components of elastic stiffness constants is 12, and 3 of them are independent components.

After computing the elastic stiffness constants, Born stability criteria [26] were checked. Those criteria can be written as follows:

$$C_{11} - C_{12} > 0;\ C_{11} + 2C_{12} > 0 \text{ and } C_{44} > 0 \quad (2)$$

As seen from Table 4, since these criteria are satisfied, MgScB is an elastically stable material.

The bulk modulus is indicative of a material's resistance to compression, while the shear modulus is defined as the ratio of shear stress to shear strain. Together, they describe the elastic behavior of the material. Three approaches can be used to calculate the bulk and shear moduli: Voigt, Reuss, and Hill. The bulk modulus gives the same results for all three approaches. While the shear modulus values from these approaches are not identical, they are very similar. According to Poisson's ratio and Pugh's ratio, this crystal is brittle. The critical values are 0.26 for Poisson's ratio and 1.75 for Pugh's ratio. If the calculated values of Poisson's ratio and Pugh's ratio are lower than the critical values, the material is considered brittle. Conversely, if the values are higher, the material is considered ductile. Since these calculated values are lower than the critical values, MgScB is a brittle material. The calculated Debye temperature value is 123.84 K. The Debye temperature was determined using fundamental physical constants, such as Planck's and Boltzmann's constants, together with material parameters including the number of molecules in the unit cell, the atomic density, and the molecular weight. These parameters were then multiplied by the calculated average sound velocity. The

calculated average sound velocity was obtained from the longitudinal and transverse sound velocities, which were obtained using the bulk modulus (B) and shear modulus (G) derived from independent elastic constants. The Debye temperature provides indirect information about lattice vibrations through its dependence on the maximum phonon frequency of the crystal. A higher Debye temperature indicates stiffer interatomic bonds and higher vibrational frequencies in the lattice; it reflects the overall vibrational energy scale of the crystal lattice. At or below the Debye temperature, high-frequency phonons are no longer active. At temperatures below the Debye temperature, only low-frequency phonons become active, and high-frequency modes are considered to be frozen [27, 28]. At temperatures above the Debye temperature, all phonon modes become active. Lattice vibrations transition to a classical behavior pattern, whereby all atoms are observed to freely share their energy.

4. Discussion and Conclusion

This study, based on density functional theory, has been carried out to determine the structural, electronic, elastic and dynamic properties of the MgScB half-Heusler crystal. The calculated lattice parameter value is quite close to the theoretical results found in the literature. To investigate the electronic structure, the electronic band structure was calculated using the lattice parameters of the calculated MgScB half-Heusler crystal. From the electronic band structure graph, the band gap of the MgScB crystal was calculated to be 0.16 eV. Since there is no similar study conducted on MgScB crystals using DFT in the literature, the results obtained in this study cannot be compared. However, the results of a previous study conducted on MgScGa, a half-Heusler crystal with properties similar to those of the MgScB crystal, can be compared. The MgScGa crystal also has a narrow band gap of 0.09 eV. Then, the total and partial density of states graphs of the half-Heusler MgScB crystal were drawn, and the results were analyzed. The phonon dispersion curve for the dynamic properties of the half-Heusler MgScB crystal was obtained. When the curve was examined, it was concluded that the MgScB crystal was dynamically stable. By performing factor group analysis for the half-Heusler MgScB crystal, the irreducible Γ representation of the MgScB crystal was obtained. Finally, the calculations performed on the elastic properties showed that the MgScB half-Heusler crystal is a brittle material. The MgScGa crystal is also brittle and dynamically stable, like the MgScB crystal. It is expected that the results of this study will provide researchers with a foundation for future studies on MgScB half-Heusler structures.

Peer-review: External, Independent.

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Declarations:

1. Statement of Originality:
This work is original.

2. Author Contributions:
Concept: SEG; ***Conceptualization:*** EKD,SEG; ***Literature Search:*** EKA,SEG; ***Data Collection:*** EKA,SEG; ***Data Processing:*** EKA,EKD,SEG; ***Analysis:*** EKA,EKD,SEG; ***Writing – original draft:*** EKA,EKD,SEG; ***Writing – review & editing:*** EKA,EKD,SEG.

3. Ethics approval:
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5. Competing Interests:
The authors declare no competing interests.

6. GenAI Usage Statement:

No GenAI tools were used at any stage of the study.

7. Sustainable Development Goals:

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