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Theoretical Study of the Electronic, Magnetic, Mechanical and Thermodynamic Properties of the Spin Gapless Semiconductor CoFeMnSi

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Abstract: CoFeMnSi has been both experimentally and theoretically proven as a novel spin-gapless semiconductor and resulted in a new research direction in equiatomic full Heusler compounds. Using the first-principles calculation method, we investigated the electronic, magnetic and mechanical properties of CoFeMnSi material in this study. The obtained lattice constant under the LiMgPdSn-type Heusler structure is 5.611 Å and it is fairly consistent with previous experimental results and theoretical calculations. Furthermore, the achieved total magnetic moment of 4 µB follows the Slater–Pauling rule as $M_{total} = Z_{total} - 24$, where M_{total} is the total magnetic moment per formula unit and Z_{total} is the total valence electron number, i.e., 28 for CoFeMnSi material. We have also examined the mechanical properties of CoFeMnSi and computed its elastic constants and various moduli. Results show CoFeMnSi behaves in a ductile fashion and its strong elastic anisotropy is revealed with the help of the 3D-directional-dependent Young's and shear moduli. Both mechanical and dynamic stabilities of CoFeMnSi are verified. In addition, strain effects on the electronic and magnetic properties of CoFeMnSi have been investigated, including both uniform and tetragonal strains, and we found that the spin-gapless feature is easily destroyed with both strain conditions, yet the total magnetic moment maintains a good stability. Furthermore, the specific behaviors under various temperatures and pressures have been accessed by the thermodynamic properties with a quasi-harmonic Debye model, including bulk modulus, thermal expansion coefficient, Grüneisen constant, heat capacity and Debye temperature. This comprehensive study can offer a very helpful and valuable reference for other relative research works.

Keywords: first principles calculation; Heusler compounds; electronic band structure; spin-gapless semiconductor; strain effect

1. Introduction

Since the discovery of spin-gapless semiconductors (SGS) from a theoretical approach by Wang, et al. [1], they immediately became interesting for the development of spintronics and magnetoelectronics [2–13]. The electronic band structure of SGS is completely spin-polarized; in one spin channel, a small band gap is present at the Fermi level, similar to in a semiconductor; whereas, in the other spin channel, the valence band maximum contacts the conduction band minimum at the Fermi level, resulting into an exactly zero gap. This particular band structure in SGS endows several special properties [1,14], such as, zero energy consumption to excite electrons from the valence band to



the conduction band, high mobility of the excited electrons, complete spin polarization of the excited electrons and holes, high sensitivity to external influence.

Among different research directions for SGSs of different structures and different components, the Heusler alloy families are particularly interesting because there are not only many theoretical calculations showing the electronic band feature of SGSs in Heusler alloys, such as Ti_2MnAl [2,12,15–17], Ti_2CoSi [5], Ti_2Vas [5], Zr_2MnAl [18,19], Zr_2MnGa [18,20] and Cr_2ZnSi [13,21,22], but also, a few experimental syntheses and measurements confirming the presence of the spin-gapless semiconducting behaviors, such as Mn_2CoAl [14], Ti_2MnAl [2]. Conventionally, Heusler compounds represent a huge family of intermetallic alloys and they can be mainly divided into two groups [23,24]: full-Heusler with general formula X_2YZ and half-Heusler with general formula XYZ, in which Z is an sp main group element and X and Y are the transition metal elements. Consequently, various Heusler compounds can be simply designed by substituting with an element from the same group in the periodic table. For a full-Heusler alloy, when the highly ordered cubic structure is considered under normal conditions, there are two typical structural configurations [12,25]: the first one is the Cu_2MnAl -type, also known as the L2₁ structure; the second one is the Hg₂CuTi-type, also known as the XA structure.

With one transition metal—element X—replaced by another transition metal—element X´—the ternary full-Heusler compounds transform into equiatomic quaternary Heusler (EQH) compounds with a change in the general formula to XXYZ [26]. The EQH compounds have a stoichiometry of 1: 1: 1: 1 and thus, the structures are less disordered [23,27–30]. Because the Mn-based and Co-based ternary Heusler materials have been investigated in numerous studies, the EQH compounds composed of Co and Mn atoms are of great interest and they can be regarded as the intermediate product of Co₂YZ and Fe₂YZ. In particular for CoFeMnZ, Dai et al. [31] firstly synthesized CoFeMnSi by an arc-melting method and confirmed its LiMgPdSb-type structure by X-ray diffraction. Different atomic orderings have been considered and, with the lowest energy configuration, it shows half-metallic properties. Afterwards, several studies followed, such as Alijani et al. [32] and Klaer et al. [33], who studied electronic, structural and magnetic properties in CoFeMnZ (Z = AI, Ga, Si, Ge) from both theoretical calculations and experimental measurements and found that there is a small amount of disorder present in the crystal structure. Then, Feng et al. [34] detailed a thorough theoretical study of the possible different disorders and their effect on the electronic and magnetic properties. Immediately after, Bainsla et al. [28] revealed the spin-gapless semiconducting behavior in EQH CoFeMnSi from experimental results. Recently, Fu et al. [35] prepared CoFeMnSi in a bulk sample and studied its magnetic and transportation properties. They found a semiconductor-like transporting characteristic in CoFeMnSi with a Curie temperature of 763 K.

While all these studies primarily investigate the electronic and magnetic properties, there are few discussions about the corresponding mechanical and thermodynamic properties. In this paper, for the purpose of providing a thorough analysis of the physical properties of EQH CoFeMnSi, we systematically investigate its electronic, magnetic, mechanical properties by first-principles calculations based on density functional theory. In addition, the effects of uniform strain and tetragonal strain are also assessed. Lastly, with the quasi-harmonic Debye model, its thermodynamic properties have also been elucidated in the temperature range 0–500 K and pressure from 0 to 10 GPa.

2. Computational Methodology

The first-principles calculations for the electronic, magnetic and mechanical properties of the Heusler compound CoFeMnSi in this work have been performed with the Cambridge Serial Total Energy Package (CASTEP) [36], which is based on the pseudo-potential plane-wave methods under the framework of density functional theory [37]. The Perdew–Burke–Ernzerhof functional of the generalized gradient approximation (GGA) [38] was selected for dealing with the electronic exchange–correlation. The ultrasoft Vanderbilt-type pseudopotentials [39] are used for the interaction between the valence electrons and the atomic core. The valence electron configurations for the four atoms are set as follows: Fe $(3d^64s^2)$, Mn $(3d^54s^2)$, Co $(3d^74s^2)$ and Si $(3s^23p^2)$. A cutoff energy of 500 eV is set for the plane-wave

basis set and a Monkhorst–Pack special $12 \times 12 \times 12 k$ sampling point mesh is selected in the Brillouin zone. The reciprocal space integrations are performed with a k-mesh of 120 points in the irreducible wedge of the Brillouin zone by using the tetrahedron method. The total energy convergence tolerance is set within 1×10^{-6} eV/atom during the self-consistent field cycle. The quasi-harmonic Debye model employed [40–42] has been adopted for studying the thermodynamic properties, and the dependencies of several parameters on pressure (0–10 GPa) and temperature (0–500 K) were computed, including unit cell volume, bulk modulus, heat capacity, Grüneisen constant, thermal expansion coefficient and Debye temperature.

3. Results and Discussions

3.1. Crystal Structure and Equilibrium Lattice

The crystal structure of the equiatomic quarternary full-Heusler compound CoFeMnSi has been both theoretically and experimentally studied [28,35] and the obtained results show it adopts the LiMgPdSn prototype cubic structure with four Wyckoff positions occupied by the corresponding four atoms: A(0,0,0) by Fe, B(1/4,1/4,1/4) by Mn, C(1/2,1/2,1/2) by Co, and D(3/4,3/4,3/4) by Si, as shown in the inset crystal structure of Figure 1. To derive the equilibrium lattice constant for CoFeMnSi in the current study, the total energy per unit cell is calculated at different lattice points and the result is displayed in Figure 1. By applying fitting and minimization of the total energies versus the lattice constants, we successfully obtained the equilibrium lattice constant of 5.611 Å at the minimum total energy point. This value is in good agreement with previous theoretical and experimental results [28,31,35].



Figure 1. The calculated total energy of CoFeMnSi with respect to different lattice constants. The inset is the corresponding crystal structure.

3.2. Electronic and Magnetic Properties

After the equilibrium lattice constant of CoFeMnSi was obtained, we calculated its electronic properties. Figure 2 shows the spin-polarized electronic band structure. It is very clear that there exists an indirect band gap (0.62 eV) in the spin-down direction, while the valence band maximum almost touches the conduction band minimum at the Fermi energy level in the spin-up channel, which reflects the spin-gapless behavior in CoFeMnSi. Although there is a small discrepancy in the band structure at the Fermi energy level, it does not affect the spin-gapless behavior as confirmed by experimental measurements. To further study the origination of the band gap in the spin-down channel, we draw a schematic diagram of the different energy levels in both spin channels for CoFeMnSi in Figure 3. It can

be seen the double degeneracy states $2 \times e_u$ are above the Fermi energy level in the spin-down channel and, thus, not occupied, leading to an $e_u - t_u$ (nonbonding - bonding) energy band gap formation. These results are consistent with a previous study [34]. According to the generalized electron filling rule and Slater–Pauling rule [43,44], the total occupied states for CoFeMnSi are 16 for the spin-up channel and 12 for the spin-down channel, respectively, and thus, a net spin magnetic moment is expected and it should be equal to 4.00 μ_B , as it is the difference between the two spin directions. At the equilibrium state, the total and partial magnetic moments are calculated and presented in Table 1. The integral value of the total magnetic moment (4 μ_B) matches the above-mentioned theoretical analysis and it follows the Slater–Pauling rule in the form of $M_{total} = Z_{total} - 24$, where Z_{total} is the total valence electron number, 28 for CoFeMnSi and M_{total} is the total magnetic moment. It can also be observed from Table 1 that Mn atoms provide the main contribution to the total magnetic moment, while Co and Fe carry relative moments aligned parallel to Mn atoma. The large magnetic moment of Mn atoms is from their strong spin-splitting effect, as revealed by the partial density of state in the literature [34].



Figure 2. The calculated spin-polarized electronic band structure of CoFeMnSi at the equilibrium lattice constant.



Figure 3. Schematic representation of the different energy levels in both spin directions for CoFeMnSi.

Compound		Lattice [Å]	Magnetic Moment [µ _B]					
			Total	Fe	Mn	Со	Si	
CoFeMnSi	Current	5.611	4.00	0.34	3.08	0.69	-0.11	
	Reference [31]	5.653 *	3.99*	0.576	2.649	0.878	-0.07	
-	Reference [28]	5.658 *	4.01	0.53	2.72	0.82		
	Reference [45]	5.67 *	3.49 *					
-	Reference [32]	5.611	4.00	0.52	2.70	0.89	-0.11	

Table 1.	The calculated equilibrium	lattice constant and	the corresponding	g total and atom-resolve	d
magnetic	r moments of CoFeMnSi.				

* Values are obtained from experiment.

To further examine the electronic bonding state and the magnetic distribution, we also calculated the distributions of the charge density difference and the electronic spin density for CoFeMnSi along the (110) plane and the results are shown in Figure 4. The electronic spin density is defined as the electron density difference between the two spin directions and the brighter color indicates a larger difference. Consequently, we can find that the large red-colored area around Mn atoms clearly indicates their strong magnetic properties, and the small area of less bright color around Co and Fe atoms indicates weak magnetism. Note that the color difference of Si atoms is indistinguishable from the background, resulting in very weak magnetism. These findings are in a good agreement with the calculated partial magnetic moments in Table 1. Regarding the charge density difference reported in Figure 4b, the blue color indicates the electron deficiency and the red color, the electron excess. The accumulation of electrons is mainly located along the diagonal directions between Fe and Co atoms, and it reflects the typical covalent bonding characteristic. A spherical blue region surrounds Si atoms, which suggests that the valence electrons of Si atoms form metallic bonds in CoFeMnSi.



Figure 4. The calculated distributions of the electronic spin density (**a**) and charge density difference (**b**) in the (110) plane of CoFeMnSi at the equilibrium lattice.

3.3. Mechanical Property and Dynamic Stability

In this section, we discuss the mechanical behavior and dynamic stability of CoFeMnSi. Only three independent elastic constants exist for a simple cubic structure and they are C_{11} , C_{12} and C_{44} , in which C_{12} and C_{44} reflect the elasticity in terms of the shape and C_{11} characterizes the elasticity in terms of the length [29,30,46,47]. All these elastic constants for CoFeMnSi have been calculated with the stress–strain method [36] and the derived values for CoFeMnSi are summarized in Table 2. By applying the Voigt–Reuss–Hill approximation [48], several other mechanical parameters, such as the bulk modulus B, the shear modulus G and the Young's modulus E, can be calculated with the following formulae as:

$$B = \frac{B_V + B_R}{2}, \ G = \frac{G_V + G_R}{2}, \ E = \frac{9GB}{3B + G}$$
(1)

where $B_V(B_R)$ and $G_V(G_R)$ stand for the lower (upper) limit of the Voigt (Reuss) boundary and they are derived from the elastic constants as follows:

$$B_{V} = B_{R} = \frac{C_{11} + 2C_{12}}{3}, \ G_{V} = \frac{C_{11} - C_{12} + 3C_{44}}{5}, \ G_{R} = \frac{5C_{44}(C_{11} - C_{12})}{4C_{44} + 3(C_{11} - C_{12})}$$
(2)

Table 2. The calculated elastic constants (Cij), bulk modulus (B), shear modulus (G), Young's modulus (E), Poisson's ratio (ν), Pugh's ratio (B/G) and anisotropy factor (η) for CoFeMnSi.

Compound		C ₁₁ [GPa]	C ₁₂ [GPa]	C ₄₄ [GPa]	B [GPa]	G [GPa]	E [GPa]	υ	B/G	η
CoFeMnSi	Current	332.2	188.9	157.5	236.7	114.8	296.5	0.29	2.06	2.19
	Reference [32]	317.0	189.0	167.0	231.0	114.0	293.0	0.29	2.04	2.60

With these values, the anisotropy factor (η) and Poisson's ratio (ν) can be also calculated as follows:

$$\eta = \frac{2C_{44}}{C_{11} - C_{12}}, \quad \nu = \frac{3B - 2G}{2(3B + G)}$$
(3)

All the values for CoFeMnSi are reported in Table 2 and it is found that the calculated elastic constants fulfill the following Born–Huang generalized elastic criteria [49,50], confirming the mechanical stability of CoFeMnSi since it has been experimentally synthesized.

$$C_{11} - C_{12} > 0, \ C_{11} + 2C_{12} > 0, \ C_{44} > 0$$
 (4)

According to the Pugh's criteria, when the Pugh's ratio of materials is smaller/larger than the critical value of 1.75, they behave in a brittle/ductile manner. In this work, the Pugh's ratio of CoFeMnSi is 2.06 and, thus, it behaves in a ductile fashion. The elastic anisotropy can be evaluated by the anisotropy factor; if it is equal to 1, the material is perfectly isotropic; if it is not equal to 1, the material is anisotropic. The calculated anisotropy factor for CoFeMnSi is 2.19 and it is bigger than 1, implying the presence of very strong elastic anisotropy. Furthermore, we also calculated the directional dependent Young's modulus and the shear modulus for CoFeMnSi; the results are reported in Figure 5 as 3D surface plots. The corresponding 2D projections in different planes are displayed in Figure 6. Note the different color curves in Figure 6 correspond to the same color curves on the 3D surface in Figure 5. The elastic anisotropy in CoFeMnSi can be clearly observed.



Figure 5. The surface plots for the calculated directional dependent Young's modulus and shear modulus of CoFeMnSi.



Figure 6. The calculated 2D projection of the Young's modulus and shear modulus of CoFeMnSi in different planes.

Dynamic stability is also very important for materials as the soft phonon modes can indicate the possible distortion in the crystal. The calculated phonon spectrum for CoFeMnSi along the high-symmetry direction (K-L-G-X-W-K) under the equilibrium lattice is shown in Figure 7. It can be clearly seen that there are no imaginary frequencies in the phonon dispersion curves, confirming the dynamic stability of CoFeMnSi.



Figure 7. The calculated phonon spectrum of CoFeMnSi.

3.4. Strain Effects

During material preparation, the distortion of the crystal structure often happens, and this situation is especially prevalent in thin-film growth. The electronic and magnetic properties are strongly related with the structures of materials and they could experience large changes under structural distortions [12,25]. Herein, we further evaluate the effects of uniform and tetragonal strains

for CoFeMnSi. It should be pointed out that the unit cell volume is maintained at the equilibrium state when the tetragonal distortion is considered.

Firstly, the effect of uniform strain is studied in terms of the electronic band structure and magnetic moments. With a uniform increase, the lattice expands and thus the distance between all atoms increases. The energy values of the valence band maximum (VBM) and the conduction band minimum (CBM) as a function of different uniform strain for CoFeMnSi in both spin-up and spin-down directions have been calculated and the result is shown in Figure 8. It is found that the VBM moves above the CBM in the spin-up direction when the uniform strain is applied, leading to the destruction of spin-gapless behavior. While for the spin-down direction, the band gap can be maintained from -5% to +1% uniform strain. Thus, even the spin-gapless feature cannot be retained with uniform strain; the half-metallicity can be considerably maintained on the negative side. When the uniform strain is above +1%, the CoFeMnSi becomes a ferromagnetic metal.



Figure 8. The calculated CBM and VBM of CoFeMnSi in both spin directions under different uniform strains.

The total and atomic magnetic moments under uniform strain are calculated and displayed in Figure 9. It is clearly shown that the total magnetic moment of CoFeMnSi stays constant—at 4 μ_B . Whereas, the magnetic moments of Mn and Fe atoms display relatively large variations under uniform strain—increase for Mn and decrease for Fe. There is a negligible change in the moment for both Si and Co atoms.



Figure 9. The calculated total and atomic spin magnetic moments of CoFeMnSi under different uniform strains.

Afterwards, the effect of tetragonal strain is further inspected with the c/a ratio from 0.9 to 1.1. The crystal changes from a cubic structure into a tetragonal structure when the c/a ratio deviates from 1. The total energy variation from the cubic structure is computed under different c/a ratios and the result is shown in Figure 10. It is found that the tetragonal distortion always increases the total energy, eliminating the possible martensitic phase transition observed in some Heusler-type compounds [46,51].



Figure 10. The calculated total energy difference of CoFeMnSi under different tetragonal strains.

The electronic band structure is examined under tetragonal strain and the variation of the CBM and VBM is shown in Figure 11. When the c/a ratio is changed from 1 to 1.02, the CBM and VBM have almost no change in the spin-up direction and thus, the spin-gapless behavior is expected to be maintained. Once a larger strain is induced, the VBM surpasses the CBM and the spin-gapless feature is lost. For the spin-down direction, the VBM moves slightly above the Fermi energy level when the c/a ratio is larger than 1.08. However, there is a band gap present in the spin-down direction, which leads to the persistence of the half-metallicity.



Figure 11. The calculated CBM and VBM of CoFeMnSi in the spin-down direction under different tetragonal strains.

The total and atomic magnetic moments under different tetragonal strains are also calculated, see Figure 12. It is observed that the total magnetic moment remains fairly constant at 4 μ_B when the

c/a ratio is varied from 0.9 to 1.1. Whereas, the partial moments of Mn and Fe atoms exhibit small variations: increase for Fe and decrease for Mn when the structure is changed from cubic to tetragonal.



Figure 12. The calculated total and atomic spin magnetic moments of CoFeMnSi under different tetragonal strains.

3.5. Thermodynamic Property

The thermodynamic properties of materials under varying temperatures and pressures can provide important information about their specific behaviors and, thus, they are of great interest. In this section, we studied the thermodynamic properties of CoFeMnSi by adopting the quasi-harmonic Debye model [12,40–42]. The variation of the normalized unit cell volume V/V₀, bulk modulus B, thermal expansion coefficient α , heat capacity C_V, Grüneisen constant γ and Debye temperature θ_D are calculated for the temperature range 0–500 K and pressure from 0 to 10 GPa.

Figure 13 shows the unit cell volume variation V/V_0 of CoFeMnSi under different pressures and temperatures. All the volumes are normalized with respect to the equilibrium volume V0 at 0 K without pressure. With increasing temperature, the cell volume continuously increases. This is apparently expected because of the thermal expansion. However, the changing rate is not constant: small at temperature from 0 to 500 K and then larger at higher temperatures. On the contrary, the cell volume continuously shrinks in a linear manner with increasing pressure due to pressure compression. Overall, the change in the volume with temperature is much smaller than with pressure under the current studied conditions.



Figure 13. The normalized volume of CoFeMnSi against different temperature and pressure.

Figure 14 displays the bulk modulus B under different temperatures and pressures. It should be mentioned here that the bulk modulus of CoFeMnSi at 0 K and 0 GPa is 230.25 GPa and it overlaps very well with the value obtained in section detailing the mechanical properties, indicating a mutual corroboration between the two different study approaches. It is observed from Figure 14 that the bulk modulus monotonously decreases with temperature increase yet increases with pressure increase. The variation follows a linear manner with pressure but shows a different rate of change with temperature: smaller when the temperature is lower than 100 K and larger at higher temperatures. This changing behavior is similar as the previous volume variation and can be instinctively understood: with increasing temperature, the compound expands and thus becomes less resistant to external compression; with increasing pressure, the compound shrinks and thus becomes more resistant to external compression.



Figure 14. The bulk modulus of CoFeMnSi against different temperatures and pressures.

The thermal expansion coefficient α of the material describes how the object size change with temperature and it is a very important parameter to study the thermodynamic equation of state. The variation of the thermal expansion coefficient α for CoFeMnSi under different temperatures and pressures is reported in Figure 15. It is shown that α changes very slightly with temperature at low temperatures, from 0 to 50 K, and then rapidly increases at higher temperatures. This finding can partially correlate to the different changing rate of volume with temperature. The change of α with temperature at different pressure shows different extents: larger variation under low pressure. With pressure increase, α shows larger variation under higher temperatures. The calculated thermal expansion coefficient for CoFeMnSi at 0 GPa and 300 K is 3.10×10^{-5} K⁻¹.



Figure 15. The thermal expansion coefficient of CoFeMnSi against different temperatures and pressures.

The heat capacity C_V is another crucial physical parameter for materials, and it can reflect important details about the lattice vibration and the phase transition. The calculated variation of C_V with pressure and temperature is depicted in Figure 16. It is clearly observed that the effect of the temperature on C_V is much stronger than that of pressure. With temperature increase, C_V slightly increases at low temperature and then grows rapidly at high temperature. With higher temperature, C_V is expected to saturate to the Dulong–Petit limit. The variation of C_V with temperature shows a very small difference among different pressures. With increasing pressure, C_V decreases slightly. The calculated heat capacity for CoFeMnSi at 0 GPa and 300 K is 80.85 J·mol⁻¹·K⁻¹.



Figure 16. The heat capacity of CoFeMnSi against different temperatures and pressures.

The Grüneisen constant γ is of great importance because it exists in several useful thermodynamic relations. The dependences of γ on pressure and temperature are plotted in Figure 17. It is observed that γ increases smoothly with increasing temperature. However, the rate of change becomes smaller at higher pressure. With pressure increase, γ decreases almost linearly and different temperatures only offset the curve vertically. The calculated Grüneisen constant of CoFeMnSi is 2.29.



Figure 17. The Grüneisen constant of CoFeMnSi against different temperatures and pressures.

The evolution of Debye temperature θ_D with temperature and pressure has been investigated and the results are shown in Figure 18. It is found that θ_D remains almost constant at the low temperature range from 0 to 100 K and then slowly decreases. The rate of change becomes smaller at higher pressure. For a given temperature, θ_D increases with pressure in a linear manner. The calculated Debye temperature of CoFeMnSi at 0 GPa and 300 K is 629.37 K. Our calculation of the thermodynamic properties of CoFeMnSi can provide a valuable reference for further work and also inspire future investigations.



Figure 18. The Debye temperature of CoFeMnSi against different temperatures and pressures.

4. Conclusions

In the current study, the electronic, magnetic and mechanical properties of CoFeMnSi have been thoroughly examined by employing first-principles calculations. Under a LiMgPdSn-type Heusler structure, the obtained lattice constant of 5.611 Å is fairly consistent with previous experiment results and theoretical calculations. The derived total magnetic moment of $4\mu_B$ obeys the well-known Slater–Pauling rule, i.e., $M_{total} = Z_{total} - 24$, with Z_{total} is the total valence electron number and M_{total} is the total magnetic moment. Moreover, the mechanical properties of CoFeMnSi have been computed under an equilibrium state and several elastic constants and moduli are obtained. It is found that CoFeMnSi behaves in a ductile manner and it exhibits very strong elastic anisotropy, as revealed by the 3D surface plots of the directional-dependent moduli. Both mechanical and dynamic stabilities of CoFeMnSi have been verified. Furthermore, the strain effects on the electronic and magnetic properties of CoFeMnSi have been investigated, including both uniform and tetragonal strains, and it is found that the spin-gapless feature is easily lost with both strain conditions yet the total magnetic moment maintains a relative good stability. Finally, the specific thermodynamic properties under various pressures and temperatures have been assessed by applying the quasi-harmonic Debye model, including bulk modulus, thermal expansion coefficient, Grüneisen constant, heat capacity and Debye temperature. The considered temperature range was from 0 to 500 K and pressure was from 0 to 10 GPa. This study comprehensively reveals different physical aspects of CoFeMnSi and can offer a very valuable reference for its real-world application.

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