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First-principles Investigations of Mechanical, and Electronic Properties of Fege

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Abstract

The mechanical and electronic properties for FeGe compound have been systematically investigated by using the first-principles calculations. The elastic constants and elastic moduli are used to reveal the mechanical properties of FeGe. The values of elastic constants and elastic moduli results show that FeGe is mechanically stable. The anisotropic constant A^U implies that FeGe is obviously anisotropic. In addition, electronic properties were calculated and analyzed. It shows that FeGe is a indirect semiconductor with a bandgap value of 0.123eV. At the same time, it has metallic behaviour. The present work present theoretical support for the further experimental investigation of mechanical and electronic properties of FeGe.

Keywords

GeFe; mechanical properties; electronic structure; first-principles calculations.

1. INTRODUCTION

The FeGe system have various polymorphs such as the hexagonal phase B-35 [1], the cubic crystal structure [2] and so on [3]. There is evidence that these compounds have many interesting properties [4]. Especially in its rich magnetic properties, it makes FeGe become an ideal magnetic material [5].

In band theory, we can obtain the explanation of the conduct of ferromagnetic materials [6]. For instance, studies have shown that the band structure of FeGe advises that the FeGe is strong enough to close the narrow gap under compression, maintaining a new magnetic ground state [7]. Therefore, we have a better understanding of the promblem's associated with FeGe by the band theory.

The unique mechanical property of FeGe also attracts great interest [8]. The elastic constants and elastic moduli are used to reveal the mechanical stability of FeGe [9].

Here, we have studied the cubic crystal structure of FeGe material, its energy band structure and elastic properties by GGA and GGA + U method. We have calculated electronic band structure and elastic constants.

2. COMPUTATION METHODS

To understand the structural, electronic, elastic property of FeGe materials, all the calculations were carried out with the first principles method based on the pseudopotential plan-wave within density functional theory (DFT). We have used Ultrasoft pseudo-potentials

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to model the ion−electron interaction. The exchange and correlation potentials were described with the generalized gradient approximation (GGA) of the Perdew-Burke-Ernzerh of form. Pseudo-atomic calculations were carried out for Fe and Ge. With cutoff energy of 400 eV and the Monkhorst−Pack special k-point scheme with 7×7×7 grid meshes in the Brillouin Zone, tests of the convergence can be obtained. The Pulay scheme of density mixing was used for the evaluation of energy and stress. At the same time, the tolerance of the geometry optimization was 5.0×10−6 eV/atom. The maximum ionic Hellmann−Feynman force, ionic displacement and stress were respectively set to be 0.01 eV/Å, 0.0005 Å and 0.02 GPa. We calculated electronic structure by the tetrahedron Bloch method with corrections. The SCF tolerance was 5.0×10−7 eV/atom. We used stress-strain method to calculated elastic constants of FeGe.

3. RESULTS AND DISCCUSION

3.1. Crystal Structure

The crystal structure of the cubic compound FeGe belongs to space group P213(No. 198) with lattice parameters of a=b=c=0.4689nm. In the unit cell of FeGe, Fe atom occupies the A(0.135, 0.135, 0.135), and Ge atom occupies the B(0.842, 0.842, 0.842), as shown in Figure 1.

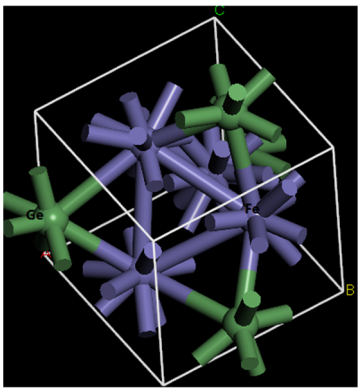

Figure 1. Crystal structure of cubic FeGe

3.2. Mechanical Properties

The cubic crystal FeGe has three independent elastic constants and C_{11}, C_{12} and C_{44} are 235.93, 110.17 and 105.16, respectively. For different elastic constants, the relationships between strain and stress of FeGe are plotted in Figure 2, Figure 3, Figure 4 and Figure 5, respectively.

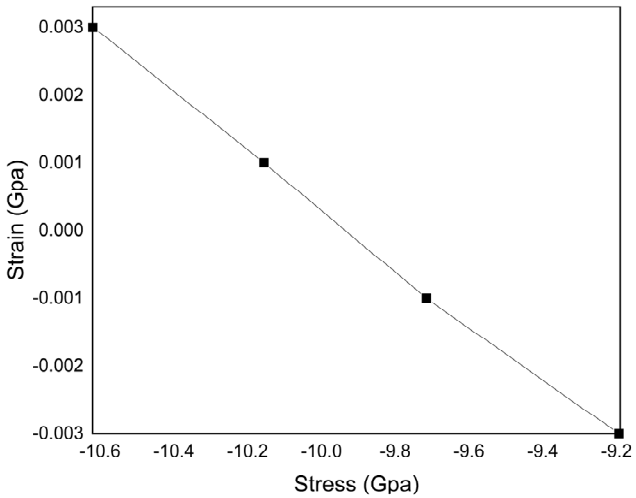

Figure 2. The relationship between strain and stress of FeGe

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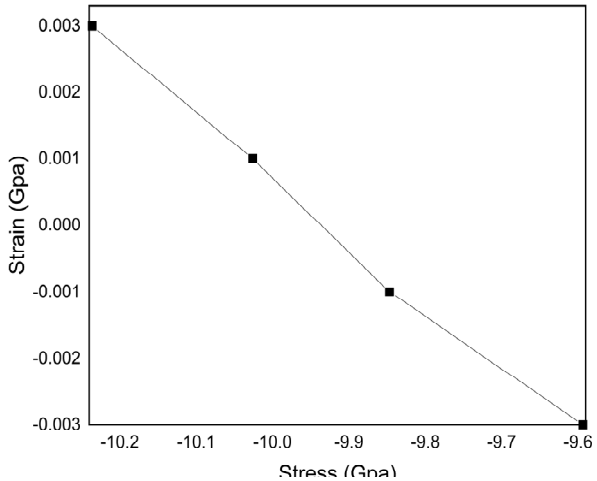

Figure 3. The relationship between strain and stress of FeGe

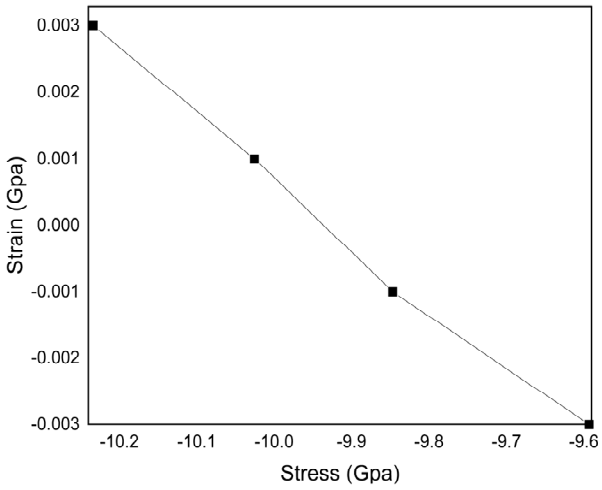

Figure 4. The relationship between strain and stress of FeGe

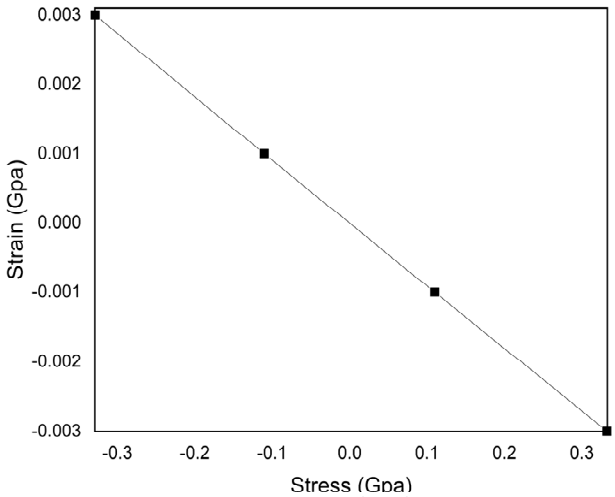

Figure 5. The relationship between strain and stress of FeGe

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These elastic constants satisfy traditional mechanical stability conditions [10], $C_{11}-C_{12}>0$, $C_{11}>0$, $C_{33}>0$, $C_{44}>0$, $C_{66}>0$, $C_{11}+C_{33}-2C_{13}>0$, $2(C_{12}+C_{11})+C_{33}+4C_{13}>0$, we can know that FeGe is mechanically stable. Because the elastic constants C_{11} and C_{33} are larger than others, FeGe is incompressible under uniaxial stress along the z axis or x axis.

We mainly use the elastic moduli to reveal the mechanical properties, where the elastic includes Poisson ratio v, shear modulus G, elastic modulus E and bulk modulus B.

The formulas of these moduli are listed as follow [11]:

$$B=\frac{1}{2}(B_V+B_R) \tag{1}$$

$$G=\frac{1}{2}(G_V+G_R) \tag{2}$$

$$v=[\frac{3B-2G}{6B+2G}] \tag{3}$$

$$E=\frac{9GB}{G+3B} \tag{4}$$

Where B_V and B_R represent the Voigt's bulk and Reuss's bulk, respectively; G_V and G_R represent the Voigt's shear modulus and Reuss's shear modulus, respectively.

According to the formulas above, we have calculated the elastic moduli to explain the mechanical property of FeGe. The calculated elastic moduli are shown in Table 1. In Table 1, the values of B and G are 148.74 and 89.36, respectively, which results in $B>G$, so the parameter limiting the stability of FeGe is the shear modulus [12]. In Table 1, we can know that the value of B/G is smaller than 1.75. This implies FeGe is the brittle material.

Table 1. Calculated elastic moduli B, G, E, v, B/G and anisotropy index A^U

B/GPa	G/GPa	E/GPa	v	B/G	A^U
148.74	89.36	223.36	0.249	1.66	0.33411

We can use the Poisson ratio v to analyze the properties of bonding forces. The upper limit and the lower limit for central force of solids is 0.5 and 0.25, respectively. As shown in the Table 1, the v value is 0.24, which is smaller than the lower limit, implying that the inter-atomic forces of FeGe are not central forces.

Elastic anisotropy constant is a significant physical parameter of materials and widely used in both industrial and technological applications. The universal elastic anisotropy index A^U are used to estimate the anisotropy of FeGe. If the A^U value of crystal is equal to zero, then it is elastically isotropic. The A^U of FeGe is 0.33411 and obviously away from 0, which implies it is anisotropic.

3.3. Electronic Properties

The electronic band structure for FeGe was calculated using approach GGA as shown in Figure 6.

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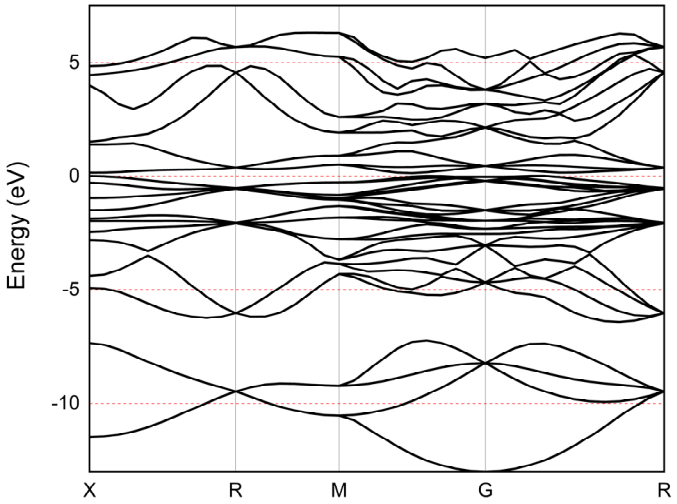

Figure 6. Band structure of FeGe

The value of band gap is 0.123eV, which implies that FeGe presents a semi-conductive character. The valance band maximum (VBM) is observed at G-R point and the conduction band minimum (CBM) is observed at M-G high symmetry k-points. This indicates that the FeGe belongs to indirect band gap. In the Figure. 6, we noticed that conduction band marginally moved to valence band in the electronic band structure and crossing Fermi level energy because of metallic behaviour of FeGe.

4. CONCLUSIONS

We have shown the mechanical, and electronic properties of the cubic crystal FeGe by the using first-principles calculations. The first, we obtained some independent elastic constants and the relationships between strain and stress of FeGe to study the mechanical properities of FeGe. We predicted that FeGe is mechanically stable and incompressible under uniaxial stress along the z axis or x axis. The second, the calculated elastic moduli which base on elastic constants, indicate that FeGe is the brittle material and it is anisotropic. At last, through analyzing the energy band of FeGe in electronic structure, it is shown that FeGe presents a semi-conductive character and belongs to indirect band gap. In addition, it has metallic behaviours.

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