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A DENSITY FUNCTIONAL THEORY ANALYSIS OF THE PRESSURE-INDUCED MECHANICAL STABILITY OF $KNiF_3$ PEROVSKITE COMPOUND

Abstract

In this study, we employed density functional theory to evaluate the structural, electronic, and mechanical properties of the $KNiF_3$ cubic perovskite compound, which belongs to the *Pm3m* space group, under high-pressure conditions ranging from 0 to 100 GPa. The results were calculated employing the GGA-PBE approximation in the Vienna Ab initio Simulation Package (VASP) code. Our findings were compared with existing research, and consistent results were obtained. The mechanical properties that our calculations determine are the following: Cauchy pressure, bulk modulus, Young's modulus, shear modulus, Pugh's ratio, Poisson's ratio, hardness, machinability index, Zener anisotropy factor, sound velocities, and Debye temperature. $KNiF_3$ compound was found to meet the criteria for mechanical stability and exhibited consistent mechanical stability across the entire 0 to 100 GPa pressure range. The computed mechanical properties suggest that $KNiF_3$ is a ductile material, and its ductility increases with pressure. The elastic anisotropic mechanical properties were visually represented. The estimation of electronic properties has been performed through spin-polarized calculations.

Keywords: *$KNiF_3$, density functional theory, structural properties, mechanical stability*

1. Introduction

$KNiF_3$ compound has a member of fluoride perovskite family, which has drawn a lot of interest in technological applications [1-11]. Despite the interest in fluoride perovskite alloys, the physical properties of the $KNiF_3$ compound have been researched poorly under pressure, to the best of our knowledge. A few experimentally measured reports on this compound's band structure [2-5]. Experimentally, Onuki et al. [2] have studied absorption spectra of KMF_3 (M=Mn, Fe, Co, Ni, Cu, and Zn) compounds. Shulman et al. [3] measured X-ray-absorption spectra of KMF_3 (M=Mn, Fe, Co, Ni, and Zn) compounds via synchrotron radiation. Using X-ray diffraction data, the topological analysis of the electron density of $KNiF_3$ were reported by Tsirelson et al. [4]. They noticed that the K-F interaction is ionic and the Ni-F bond shows polar covalent type in $KNiF_3$. Rousseau et al. [5] were reported on the elastic constants of perovskite AMF_3 (A =K, Rb; M=Mg, Ni, Co, Zn, Mn) compounds by long waves method. Kitamura et al. [6] studied electronic properties of KMF_3 (M = Mn, Fe, Co, Ni, Cu, and Zn) compounds.

The electronic properties, magnetic properties and elastic properties of $KNiF_3$ has been obtained by Ref [7] using the ab initio method within Hartree-Fock approach as implemented in the CRYSTAL code. They found that $KNiF_3$ is a large gap insulator in ferromagnetic and antiferromagnetic phase [7]. Pari et al. [8] is theoretically investigated antiferromagnetic electronic structure of title compound. Moreira et al. [9] studied the magnetic coupling of $KNiF_3$ via an ab initio method within cluster model approach. Erum and Iqbal [10] calculated the elastic, optic and magneto-electronic features of $KNiF_3$ via an ab initio method. They point out that $KNiF_3$ compound shows ductile and anisotropic characteristic. The first principle calculation of electronic and magnetic properties for title compound is also reported in Ref [11] using WIEN2K package. They reported $KNiF_3$ compound is elastically stable in Pm3m space group.

2. Materials and Methods

In this study, the properties being investigated include structural, electronic, elastic, and related properties of the $KNiF_3$ compound were obtained using first-principles calculations within Vienna Ab-initio Simulation Package (VASP) [12]. The study covers a pressure range from 0 to 100 GPa.The interaction between valence electrons and ionic cores is modeled using the projector augmented-wave (PAW) [13, 14] approach. The generalized gradient approximation (GGA) is employed for the exchange-correlation energy. Specifically, the Perdew-Burke-Ernzerhof (PBE) functional is used [15]. The number of k-points was set to Monkhorst-Pack [16] scheme 16 x 16 x 16 after the convergence test, and the cut off energy was 700 eV. These numbers were sufficient to satisfy convergence criterion for $KNiF_3$ compound.

3. Results and Discussion

3.1. Geometric optimization

By employing fully geometrical relaxation, the predicted $KNiF_3$ lattice parameters are obtained. Table 1 present the computed values of lattice constant (a_0) with experimental and theoretical value. The experimental lattice constants coincide quite well our prediction. The pressure effect of lattice constant for this compound is depicted in Figure 1. It is shown clearly that lattice constant of $KNiF_3$ is decreased by increasing the pressure. This can be expressed that there exist stronger atomic interactions. Unfortunately, unavailability of theoretical or experimental results, the ambient pressure values of calculated lattice constants cannot be compared.

Table 1. Calculated structural equilibrium lattice constant a_0 (in Å) of $KNiF_3$.

$KNiF_3$	$\boldsymbol{a_0}$ **(Å)**
Present-PBE	4.039
Experimental [5]	4.010
Experimental [17]	4.034
Theory [7]	4.10
Theory [8]	4.12
Theory [10]	4.013^{LDA} 4.018^{GGA}
Theory [11]	4.012

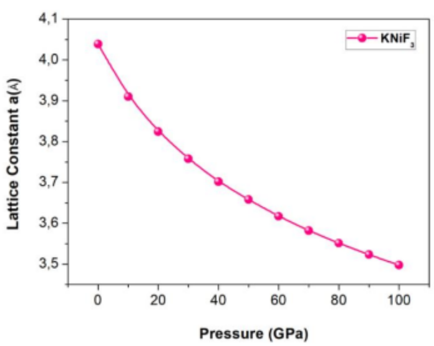

Figure 1. Pressure dependence of lattice constant of $KNiF_3$.

3.2. Mechanical stability

Through application of the "stress-strain" method [18], the mechanical properties of cubic perovskite $KNiF_3$ under high pressure are characterized by three independent elastic constants: C_{11}, C_{12}, and C_{44}. Table 2 shows the computed C_{ij} of $KNiF_3$ at P = 0 GPa. According Table 2, our predicted elastic constant values at 0 GPa correspond well with the published experimental values [5]. Thus, our calculation approach is plausible and accurate. The results obtained at 0 GPa also agree with prior theoretical studies in general [7, 10, 11]. The elastic constants of the title compound rise with increasing pressure, as shown in Figure 2. It's also worth noting that under 100 GPa, the obtained C_{11}, C_{12}, and C_{44} are all positive and fullfill the requirements [19] for the cubic structure. It's also found that C_{11} is more susceptible to pressure than C_{44} which has the least effect.

Table 2. Elastic properties of $KNiF_3$ at 0 GPa.

$KNiF_3$	Present- PBE	Exp. [5]	Theory [7]	Theory [10]	Theory [11]
C_{11} (GPa)	140.96	158.2	168	121.231	115.73
C_{12} (GPa)	54.771	48.5	60	58.989	53.85
C_{44} (GPa)	36.278	40.3	46	46.639	41.63
Cauchy Pressure (GPa)	18.49			12.06	
B (GPa)	83.50		79	80.217	89.26
G (GPa)	38.87			39.971	36.96
Y (GPa)	100.94			102.824	95.14
B/G	2.15			2.006	2.01
ν	0.299			0.29	0.2
μ_M	2.30				
A	0.84			1.55	1.35
H_v (GPa)	5.15				
v_l (m/s):	5890.22			5440	
v_t (m/s):	3156.71			2980	
v_m (m/s):	3525.32			4210	
θ (K)	444.3			320	

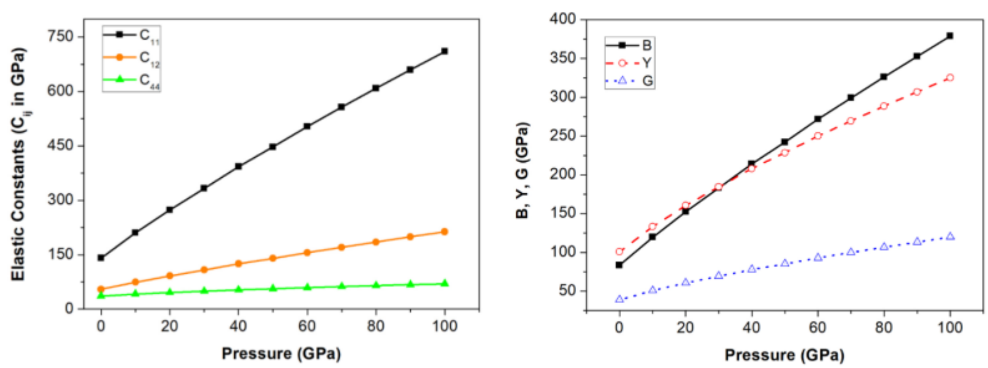

Figure 2. Pressure dependence of elastic properties of $KNiF_3$ compound.

Furthermore, various additional mechanical properties, such as Cauchy pressure, bulk modulus (B), shear modulus (G), Young's modulus (Y), machinability index (μ_M), Zener anisotropy factor (A), Poisson's ratio (ν), Pugh's ratio (B/G), hardness (H_v), longitudinal wave velocity (v_l), transverse wave velocity (v_t), average wave velocity (v_m), and Debye temperature (θ) were systematically calculated [20-27]. The corresponding values of these mechanical properties at 0 GPa are provided in Table 2, and their pressure dependence is illustrated in Figure 2. The bulk modulus (B), shear modulus (G), and Young's modulus (Y) exhibit an upward trend with increasing pressure within the specified pressure range.

Table 2 shows that the B/G ratios of $KNiF_3$ are more than 1.75, indicating that it is ductile [24, 25]. At 0 GPa, the B/G value of the title compound changes from 2.15 to 3.16 at 100 GPa. This suggests that as the pressure is increased, the $KNiF_3$ becomes more ductile. Cauchy pressure is found 18.49 GPa at zero pressure and 143.3 GPa at 100 GPa pressure. These values exhibit ductile nature and ductility of this compound increase also with pressure. The ductility of this compound is also confirmed since the obtained value of ν is bigger than 0.26 [10, 25]. The elastic ansitropy properties [28] is also depicted in Figure 3 and 4.

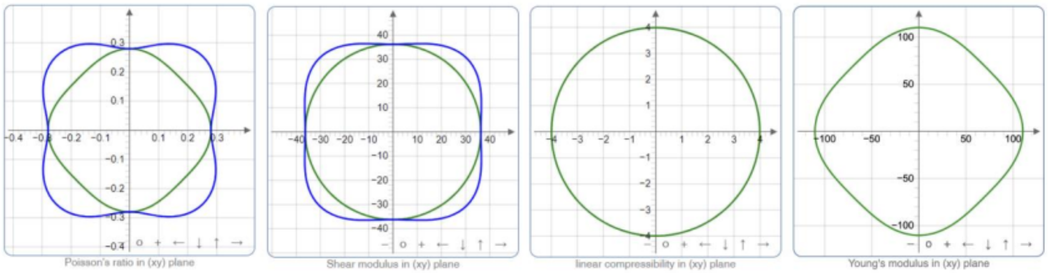

Figure 3. 2D elastic anisotropy properties of $KNiF_3$ compound at 0 GPa.

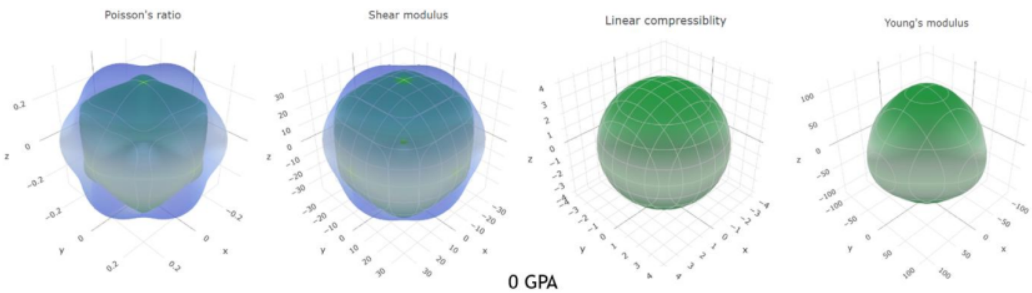

Figure 4. 3D elastic anisotropy properties of $KNiF_3$ compound at 0 GPa.

3.3. Electronic properties

The electronic properties were determined using spin-polarized calculations. The spin-up and spin-down electronic band structure presentation for $KNiF_3$ compound is given in Figure 5 and and total density of states (TDOS) is displayed in Figure 6. The computed electronic band structure aligns with the existing theoretical findings [10, 11] at 0 GPa.

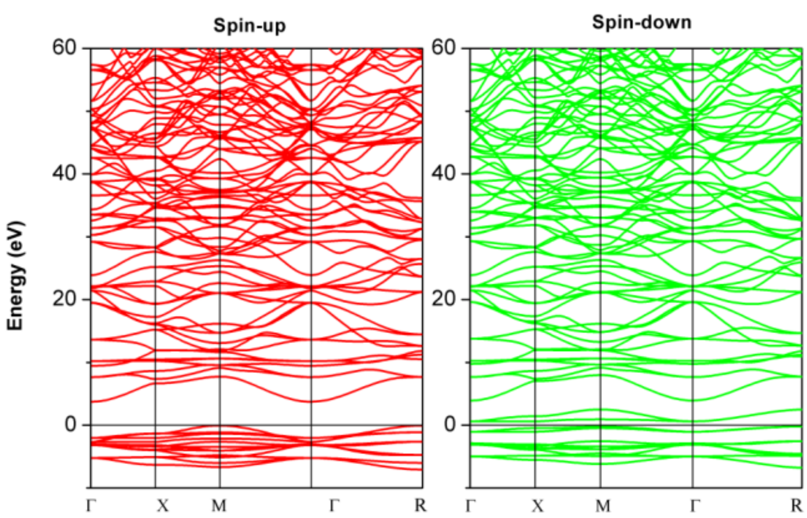

Figure 5. Electronic band structure of $KNiF_3$ compound at 0 GPa.

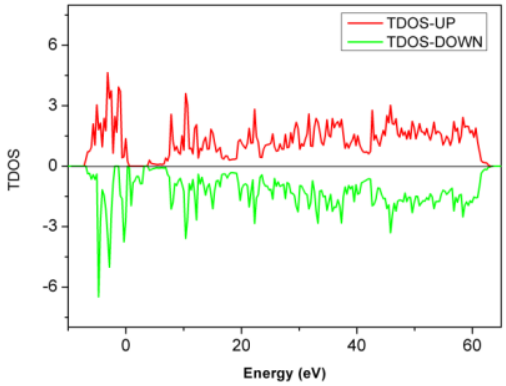

Figure 6. Total density of states of $KNiF_3$ compound at 0 GPa.

4. Conclusion

This study employed first principles calculations to investigate the impact of pressure (in the range of 0–100 GPa) on the physical properties of fluoroperovskite $KNiF_3$ compounds. The lattice constant, spin polarized electronic band structure, and elastic constants presented in this research consistent with both experimental structures and theoretical studies. The findings reveal a reduction in lattice constants under pressure, accompanied by an increase in elastic constants as the pressure rises. Importantly, at the assessed pressure levels, all elastic constants adhere to the conditions for mechanical stability.

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