Mechanical and Anisotropy Properties of Trigadolinium Heptanickel Tetradecaaluminide ($Gd_3Ni_7Al_{14}$) Compound

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Abstract: $Gd_3Ni_7Al_{14}$ compound is in the hexagonal P-62m structure. We have studied the structural, electronic, elastic and anisotropy properties. We have been used strass-strain method to predict the second order elastic constants (C_{ij}) of the titled compound within the density functional theory. Our results showed that the compound is satisfy mechanical stability for the considered structure. The polycrystalline aggregate behavior estimated using the elastic constants. The bulk modulus, shear modulus, Young's modulus, Possion's ratio, Debye temperature, and anisotropy value of polycrystalline aggregates have been derived and relevant mechanical properties are discussed.

Keywords: $Gd_3Ni_7Al_{14}$, mechanical properties, anisotropy properties.

1. Introduction

Gd-Ni-Al system has been investigated by Rykhal et. Al. Since that, many ternary intermetallic Gd-Ni-Al compounds confirmed [1]. Some of them crystalized in orthorhombic ($GdNiAl_4$, $GdNiAl_2$, $Gd_3Ni_5Al_{19}$ and Gd_2Ni_2Al), in hexagonal (Gd_3Ni_8Al, $GdNi_2Al_3$, $GdNi_3Al_9$ and GdNiAl), in cubic (Gd_3Ni_6Al2), and in monoclinic ($Gd_4Ni_6Al_{23}$).

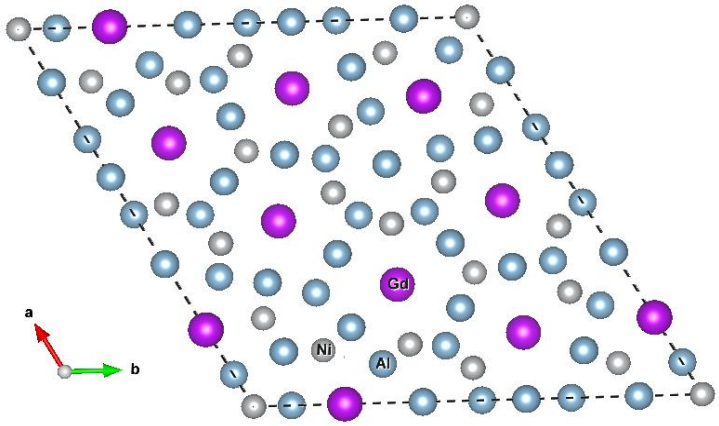

Figure 1. The crystal view of hexagonal $Gd_3Ni_7Al_{14}$ compound.

$Gd_3Ni_7Al_{14}$ was synthesized and analyzed by Pukas and Gladyshevskii [2]. Its structure belongs to Hexagonal (P-62m, Z=3) (See Figure 1). There is not enough information about the physical properties of this compound. Therefore, we performed the systematic density functional theory (DFT) investigation of structural, mechanical, and anisotropic properties of the Trigadolinium Heptanickel Tetradecaaluminide ($Gd_3Ni_7Al_{14}$) compound to fill this gap. The organization of this study is as follows: The method of calculation is given in Section 2, the results and overall conclusions are presented and discussed in Section 3.

2. Method

The calculations were carried by using the VASP code [3-4] based on DFT. The electron–ion interaction was considered in the form of the projector-augmented-wave (PAW) method with plane wave up to an energy of 400 eV [5], an adequate value for studying the physical properties. Perdew–Burke–Ernzerhof (PBE) type functional [6] within the generalized gradient approximation (GGA) has been used for the exchange and correlation terms in the electron–electron interaction. 4x4x11 Gamma centered k-mesh grid (with ~0.1 $Å^{-1}$ grid space) has been used [7]. The second order elastic constants (C_{ij}) were obtained using The stress-strain method implemented in the VASP code [8].

3. Results and Discussion

3.1. Structural properties

$Gd_3Ni_7Al_{14}$ compound belongs the hexagonal P-62m structure (Space Group No:189, Z=3) [2]. The structural view of the titled compound is given in Fig. 1. The x-ray diffraction data [2] were used as an input for energy minimization. The calculated lattice parameters, ground state energy E_0 and volume are listed in Table 1. Our results for the titled compound agree well with x-ray observations. We were used the optimized parameters for the subsequent calculations.

Table 1. The calculated lattice parameters (a, c in Å), ground state energy (E_0 in eV/fu), and volume (V_0 in $Å^3$/uc) with available experimental values.

	a	***c***	***E_0***	***V_0***	***Ref.***
	18.0301	4.0497	-148.46	1140.12	Present
	17.966	4.0448		1130.60	Exp. [2]
Percentage deviation	%0.36	%0.12		%0.84	

3.3. Mechanical properties

3.3.1. Elastic constants

We have used the “stress-strain” relations [8] to carry out the six second order elastic constants (C_{ij}) for hexagonal systems, and the determined values are given in Table 2. The results satisfy the Born mechanical stability criteria ($C_{11}>0$, $C_{44}>0$, $C_{11}- C_{12}>0$, $(C_{11} + C_{12}) C_{33}-2 C_{12}^2>0$) [9, 10] for hexagonal crystals. It shows that the compound is mechanically stable.

Table 2. The calculated elastic constants (C_{ij} in GPa unit).

Compound	***C_{11}***	***C_{12}***	***C_{13}***	***C_{33}***	***C_{44}***	***C_{66}***
$Gd_3Ni_7Al_{14}$	193.6	54.8	65.8	222.2	79.4	69.4

The polycrystalline mechanic modules, such as bulk modulus (B), Young’s modulus (E), shear modulus (G), Poisson’s ratio (v) and shear anisotropy factor (A) which are

functions of the elastic constants, are calculated by using the Voigt–Reuss–Hill approximation [12, 13], and are listed in Table 3.

Table 3. Calculated bulk modulus (B in GPa), isotropic shear modulus (G in GPa), Young's modulus (E in GPa), Vicker Hardness (H_v in GPa), Poisson's ratio (v), B/G ratio, the percentage of anisotropy in the compression and shear (A_B, A_G in %), and the universal anisotropy factor (A^u).

B	**G**	**E**	**H_v**	**v**	**B/G**	**A_B**	**A_G**	**A^u**
108.7	73.6	180.1	12.7	0.22	1.48	0.4	0.3	0.032

Bulk, shear, Young's and hardness values indicates that it is hard material. According to criterion, a material is brittle (ductility) if the B/G ratio is less (high) than 1.75. The calculated value of the B/G (1.48) is less than 1.75 for the titled compound; hence, the compound will behave in a brittle manner.
The typical value of Poisson's ratio gives information about bonding. In the present case the value of v is 0.22 shows that the ionic contributions to the atomic bonding are dominant for the titled compound.

For a completely isotropic material, the factor A^u takes the value of zero. When the value of A^U is greater than that, it is a measure of the degree of elastic anisotropy. The results show that the compound has very little anisotropy. Also, it has little percentage Bulk and shear moduli (~%0.3).

3.3.2. Anisotropic Properties

We also calculate and visualize the spatial dependence of the Young's modulus, linear compressibility, Shear modulus, and Poisson ratio by using ELATE code [14, 15]. In the plots of these physical properties, the degree of anisotropy is indicated by the deviation from the spherical shape. These parameters along the crystallographic directions (in 2D) have been given in Figure 2 for $Gd_3Ni_7Al_{14}$ compound. It is showed that all modulus in *xy*-planes exhibiting to be more isotropic than the others. For xz- and yz-plane, the material has little anisotropy.

4. Conclusion

In summary, we have performed the first principles total energy calculation for $Gd_3Ni_7Al_{14}$ using the plane-wave pseudopotential approach to the density-functional theory within the generalized gradient approximation. The calculated lattice parameters are consistent with the literature values. The B/G ratio is 1.48 and the brittle character is dominant. The titled compound has a little elastic anisotropic character. We hope that our other predicted results will be serving as a reliable reference for the future experimental and theoretical studies.

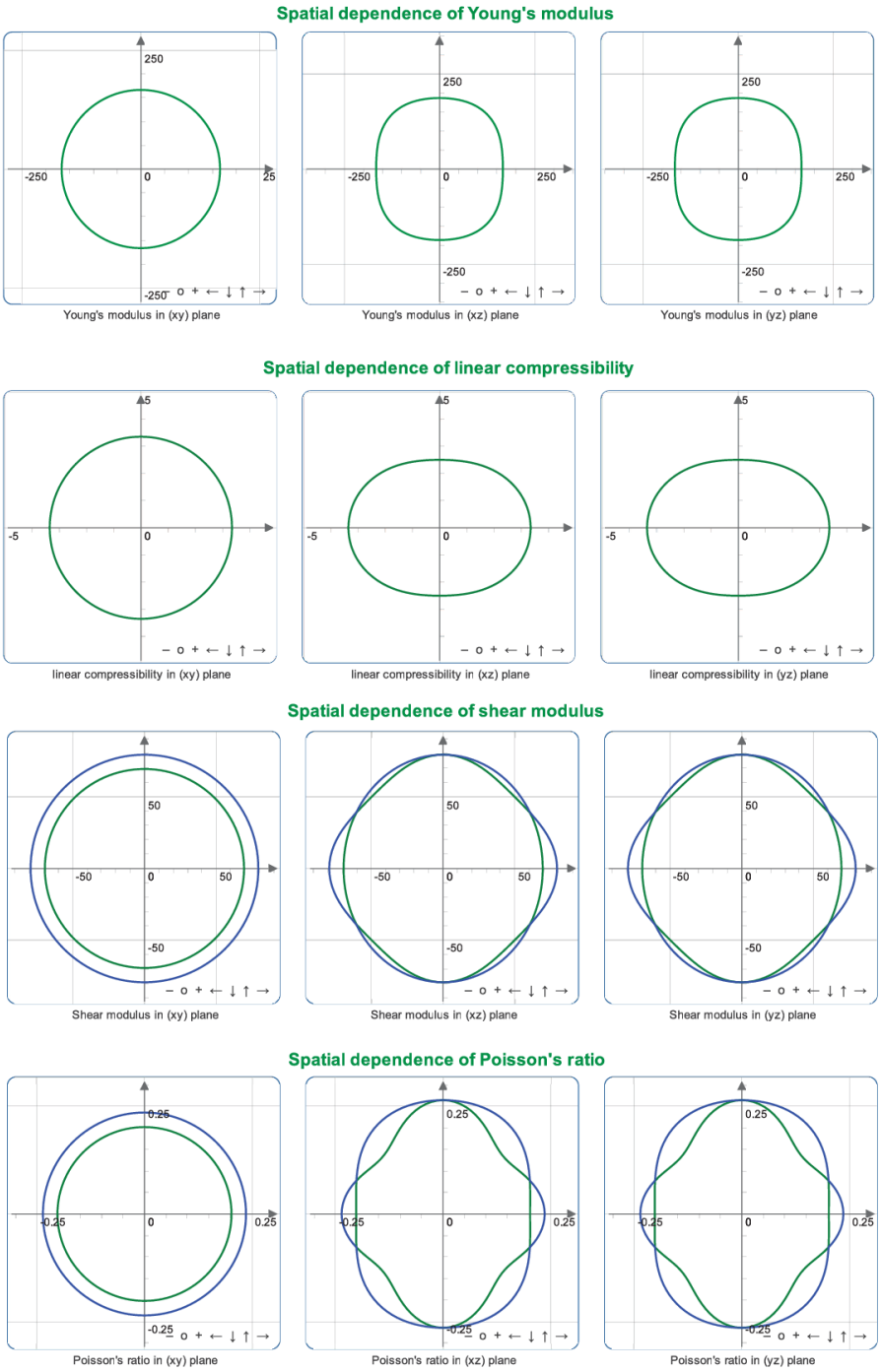

Figure 2. The calculated spatial dependence of the polycrystalline mechanical modulus.

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