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Elastic properties calculation of Hexagonal Gallium Nitride doped with Osmium in the presence of Universal force field

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Abstract. Hexagonal GaN is a wide band gap semiconductor of group III/V. It has different applications in the field of laser, storage device, telecommunications etc. In this present work, investigations on the elastic properties of Osmium doped hexagonal GaN is done using the universal force field by DFT method. As the GaN shows the brittle nature, sometimes it is hard to fabricate in a device. So the main motivation of the work to reduce the brittleness of the GaN by doping the malleable and ductile Osmium metal. Osmium metal is corrosion resistive with high melting point. Here various elastic parameters of hexagonal GaN like young's modulus Y, bulk modulus B, compressibility K, Poisson's ratio σ, shear modulus G calculated on Universal force field using Density functional theory for Os doped GaN at Ga-site as well as N-site. Also processed the elastic stiffness constants 6×6 matrix in an elastic tensor analysis (ELATE) software for the 3D illustrations of the various elastics constants.

Keywords: GaN, DFT, Osmium, Elastic property, Elastic constants, ELATE, Forcite, Universal Force field

1. Introduction

The brittleness of the material does not favour in the process of fabrication of the GaN laser. Scientists, researchers and engineers searching of a good material which after doped with GaN can improved the ductility, electrical, optical and magnetic properties as well. Lustrous and silvery Osmium metal which used in space industry for its high reflectivity can be doped with Hexagonal GaN to reduce the brittleness of the GaN. Osmium is a ductile and malleable metal having high melting points. Wide bandgap Hexagonal wurtzite GaN semiconductor of (3.4eV) used for transistors, diodes, LEDs, lasers etc. Few works related to Graphene structured GaN (g-GaN) using hybrid functional

investigated [1]. In this paper, elastic properties of Osmium doped hexagonal GaN computed at Ga-site as well as N-site. Computational work on Elastic constants like young's modulus, bulk modulus, shear modulus, compressibility, Poisson's ratio derived and analysed for applications. Stiffness constants Cij (GPa) and Compliance constants Sij (1/TPa) of 6×6 elasticity matrix calculated for Os doped GaN using the Forcite module of Biovia material studio [4,5]. Elastic Tensor Analysis (ELATE) software processed the Stiffness matrix Cij and illustrated the 3D cartoons of elastic constants [6-11]. C_{11}, C_{12}, C_{13}, C_{33}, C_{44}, C_{66} unconstrained elastic constants evaluated. Using different theorem, we analyses for different properties like hardness, brittleness, ductility anisotropic property etc.

2. Computational Methods

First principle energy code Biovia material studio uses for theoretical calculations of the various properties of the materials. Here material studio Forcite module used for the calculations of the elastic properties of the substance. For structure of the primitive Hexagonal GaN, P63MC space group [12] used with lattice specifications of a=b=3.216Å c=5.240 Å and α=β=90 γ=120 taken. Forcite calculation for the optimisation of the structure uses the smart algorithm of energy 1.0×10^{-4}kcal/mol. After applying the constant strain of 3×10^{-3}, the optimised structure of hexagonal GaN changed lattice specifications to a=b=3.0941 Å c=5.0348 Å. Universal force field [2,3] applied for the periodic table elements to calculate the mechanical properties. Periodic system's long range interaction computed by Ewald electrostatic summation method. Atom based Vander Waals interaction considered and cubic spline Truncation method is used. Single and double Osmium atom doped at different Ga-site as well as N-site of hexagonal GaN.

3. Results and Discussion

Dassault systems Biovia Forcite module is a nifty mechanical tools which provides us reliable geometry optimization with fast calculations of different mechanical properties. Forcite calculations depends on the force field. Here universal force field apply to calculate the mechanical and elastic properties of the hexagonal GaN. Bonding characteristics of the adjacent planes of the atom, stiffness, stable structure configuration and the anisotropic bonding nature data provides the characteristics elastic properties of the Hexagonal GaN. The Forcite calculation with universal force field provides the stiffness constants Cij (GPa) [13] and compliance constants Sij (1/TPa) [14] for the hexagonal GaN.

For calculations of elastic constants, an expansion of Taylor series of energy which is a function of lattice strain considered.

Table 1. Six unconstrained elastic constants Cij (in GPa), elastic compliance constants Sij and shear anisotropic factors A [15]

	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	C_{66}	S_{11}	S_{12}	S_{44}	A
Pure GaN	592.37	100.72	83.88	721.33	229.19	245.82	1.7593	-0.2747	4.3633	1.073
Os doped at Ga-site	588.67	114.82	103.89	705.12	221.52	236.91	1.7984	-0.3122	4.5146	0.935
Os doped at N-site	562.35	116.33	100.97	684.47	205.61	223.00	1.8916	-0.3505	4.8637	0.921
2Os doped at Ga-site	586.55	118.53	131.01	698.55	207.74	225.24	1.8326	-0.3034	4.8187	0.887
2Os doped at N-site	532.11	125.53	121.25	650.68	176.13	198.09	2.0466	-0.4062	5.6826	0.866

For stable structure, the Born Huang criteria [16] must follow by the six unconstrained elastic constants Cij as follows: $C_{11} > 0$; $C_{33} > 0$; $C_{44} > 0$; $C_{66} > 0$; $C_{11} - C_{12} > 0$; $(C_{11} + C_{33} - 2C_{13}) > 0$; $2[(C_{11} + C_{12}) + C_{33} + 4C_{13}] > 0$

All the Borne Huang criteria satisfies in the case of Osmium doped hexagonal GaN. Hence Osmium doped hexagonal GaN is a stable structure. For GaN semiconductor and the Osmium doped GaN, the compliance constants and the stiffness constants are linked by

$$S_{11} = \frac{1}{3}\left(\frac{1}{C_{11}+2C_{12}} + \frac{2}{C_{11}-C_{12}}\right);\ S_{12} = \frac{1}{3}\left(\frac{1}{C_{11}+2C_{12}} - \frac{2}{C_{11}-C_{12}}\right);\ S_{44} = \frac{1}{C_{44}}$$

Table-1 shows all the independent elastic constants .The value found to be positive and also satisfies the Borne Huang criteria. This implies that GaN semiconductor doped Osmium compound is stable mechanically. Elastic anisotropy depends upon the orientation of the elastic modulus. Also Elastic anisotropy depends upon the sound velocities in the plane of the lattice.

Anisotropic factor relates with the independent elastic constants

$$A=\frac{2C_{44}}{C_{11}-C_{12}}$$

For isotropic, the A value is equal to be 1. If the value of A is less or greater than the value of 1, then the studied material is an anisotropic is nature. Clearly, hexagonal GaN is an anisotropic elastic in nature.

In Voigt approximation, the bulk modulus Bv and the shear modulus Gv represented [17] as

$$B_v=\frac{1}{9}[2(C_{11}+C_{12})+4C_{13}+C_{33}]$$

$$G_v=\frac{1}{30}(C_{11}+C_{12}+2C_{33}-4C_{13}+12C_{44}+12C_{66})$$

In Reuss approximation, the bulk modulus B_R and the shear modulus G_R represented [18] as

$$B_R=\frac{(C_{11}+C_{12})C_{33}-2C_{13}^2}{C_{11}+C_{12}+2C_{33}-4C_{13}}$$

$$G_R=\frac{5C_{44}C_{66}[(C_{11}+C_{12})C_{33}-2C_{13}^2]}{2[3B_V C_{44} C_{66}+\{(C_{11}+C_{12})C_{33}-2C_{13}^2\}(C_{44}+C_{66})}$$

In Hill approximation, the bulk modulus B and the shear modulus G represented [19] as

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

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

Young's modulus Y and Poisson's ratio σ relates by

$$Y=\frac{9BG}{3B+G}$$

$$\sigma=\frac{3B-2G}{2(3B+G)}$$

Table 2. Estimated Bulk modulus (BR, Bv, B in GPa), Shear modulus (GR, Gv, G in GPa), Young's modulus (Y in GPa), Compressibility (K in GPa-1), G/B and Poisson's ratio σ.

	B_R	B_V	B	G_R	G_V	G	Y	K	G/B	σ
Pure GaN	269.9	271.5	270.7	247.3	250.0	248.7	571.1	0.0037	0.919	0.1483
Os doped at Ga-site	279.4	280.9	280.1	237.8	239.9	238.9	558.1	0.0035	0.852	0.1679
Os doped at N-site	270.2	271.8	270.9	223.5	226.2	224.9	528.5	0.0037	0.829	0.1749
2Os doped at Ga-site	289.1	290.5	289.8	227.8	230.5	229.1	544.0	0.0034	0.791	0.1871
2Os doped at N-site	270.0	271.5	270.7	196.4	200.5	198.4	478.4	0.0037	0.732	0.2055

Estimated Bulk modulus (BR, Bv, B in GPa), Shear modulus (GR, Gv, G in GPa), Young's modulus (Y in GPa), Compressibility (K in GPa-1), G/B and Poisson's ratio σ shown in Table-2 for pure GaN and different concentration of the Osmium doped on GaN at Ga-site as well as N-site.

Materials is ductile on the basis of Pugh's criteria [20], If G/B < 0.5. Here the G/B > 0.5 which shows the brittle nature of the Os doped hexagonal GaN. Also Poisson's ratio is very low which shows the brittleness of the material. But with increasing percentage of the Osmium metal, the brittleness reduces. Further studying required for the percentage of doping increases or will go for suitable co-doping material for ductility increase in GaN. Poisson's ratio increases with the increasing of doping material percentage. After processing the Elastic stiffness constants Cij in elastic tensor analysis (ELATE) software ,3D plot of the Poisson's ratio, Young's modulus, linear compressibility, Shear modulus of Hexagonal GaN done.

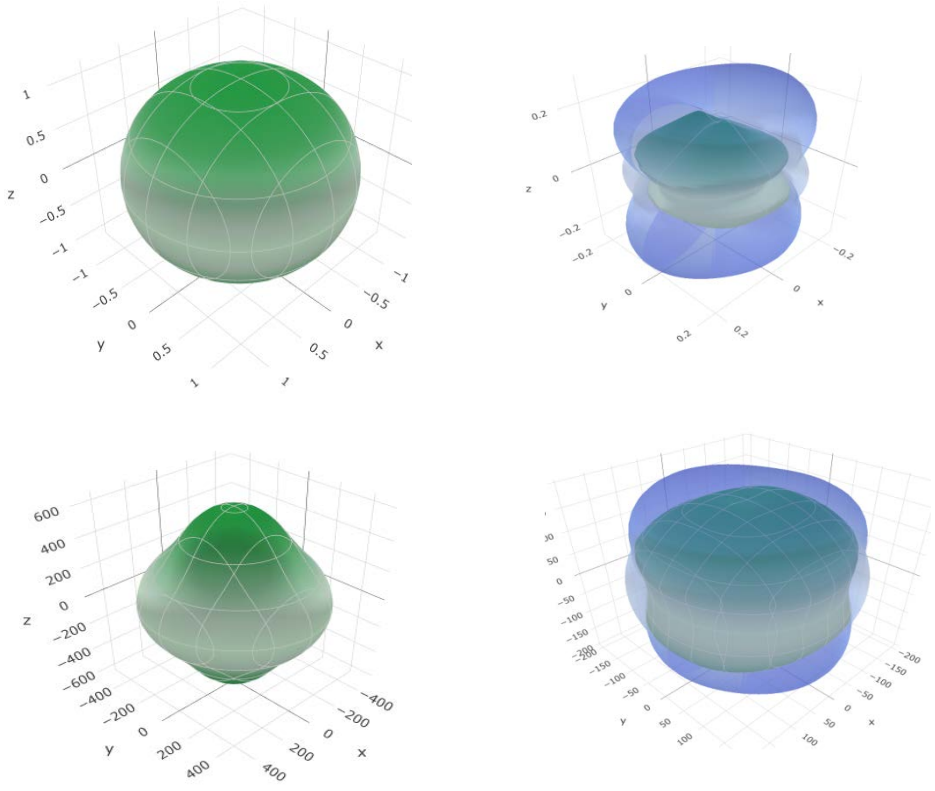

Fig. 1. 3D plot of the Young's modulus, Poisson's ratio, linear compressibility, Shear modulus of Two Osmium atom doped at N-site of Hexagonal GaN

4. Conclusion

Elastic properties calculations done for the Osmium doped hexagonal GaN using density functional theory in Forcite module of Biovia material studio. Universal force field applied for the elastic constants calculations. Computed Young's modulus, Shear modulus, Bulk modulus, G/B ratio, Poisson's ratio for the Osmium doped GaN at Ga-site as well as N-site. From the G/B ratio and the low Poisson's ratio, the osmium doped hexagonal GaN found to be brittle but the brittleness reduces with the increase percentage of Osmium metal doping. With further doping and co-doping of different materials can be reduces the brittleness of the material which is a matter of rigorous research and computational work.

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