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First-principles investigation of mechanical and electronic properties of tetragonal $NbAl_3$ under tension

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ABSTRACT

Using the density functional theory calculations, the mechanical and electronic properties of $NbAl_3$ under different tensile loads were investigated. The calculated lattice parameters, elastic constants and mechanical properties (bulk modulus, shear modulus, Young's modulus, Poisson's ratio, Pugh's criterion and Cauchy's pressure) indicated that our results were in agreement with the published experimental and theoretical data at zero tension. With respect to $NbAl_3$ under tension in this paper, the crystal structure was changed from tetragonal to orthorhombic under tension along the [100] and [101] directions. The $NbAl_3$ crystal has been classified as brittle material under tension from 0 to 20 GPa. The obtained Young's modulus and Debye temperature monotonically decreased with increasing tension stress. Combining with mechanical and electronic properties in detail, the decreased mechanical properties were mainly due to the weakening of covalency.

1. Introduction

With the development of high thrust-weight ratio engines, the $NbAl_3$ intermetallic with comparatively high stiffness, low density, high melting point and high creep strength attracts much attention [1–5]. However, as a high-temperature structural material for turbine blades and combustion chambers, the $NbAl_3$ crystal with $D0_{22}$ structure has barriers to the practical applications [6–8]. Among the barriers, the major restriction is its room temperature brittleness [9–11]. Besides, the low ductility and low toughness which are related to the lower symmetry and less slip bands [10,12–15] also hinder its developments.

It is well known that the brittle fracture occurs when the rheological pressure is greater than the cleavage stress. Hence, the brittleness can be improved with reducing the flow stress by alloying. The improvement in strength can be completed by rapidly solidified and hot isostatic pressing $NbAl_3$+1%TiB_2 [16]. The fracture toughness, high-temperature strength and brittle-to-ductile transition temperature (BDTT) could be controlled by changing the contents of $NbAl_3$, NiAl and NbNiAl [17]. The strength and toughness can be improved by incorporating the WHfC filaments [18]. In addition, the deformation modes and grain size softening effect in $NbAl_3$ were found [19,20]. The fracture toughness of polycrystalline, hardness properties of Al-$NbAl_3$ were also studied in experiments [21].

It can be seen that many works have been devoted to mechanical properties of $NbAl_3$, e.g. the improvements of strength and ductility. However, to the best of our knowledge, these mechanical properties under tension have not been reported. Hence, in this paper, the mechanical and electronic properties under tension along different crystallographic orientations have been investigated by the pseudo-potential plane wave method.

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Table 1
Calculated elastic constants (C_{ij}, GPa), bulk modulus (B, GPa), shear modulus (G, GPa), Young's modulus (E, GPa), Poisson's ratio (ν), B/G and Cauchy's pressure (GPa) of tetragonal $NbAl_3$ under zero tension.

	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	C_{66}	C_{12}-C_{44}	B	G	E	ν	B/G
This work	246.6	96.3	48.5	272.8	104.4	138.3	−8.1	128.0	105.5	248.3	0.177	1.213
PW91 [8]	230.6	71.6	44.5	259.5	94.0	123.2	−22.4	115.8	98.5	230.2	0.169	1.175
PW91 [11]	255.6	101.4	51.2	274.8	104	140.5	−2.6	132.5	106.5	252	0.183	1.244
PBE [12]	260.19	96.72	46.53	280.27	109.94	142.46	−13.22	131.00	111.34	260.28	0.17	1.18

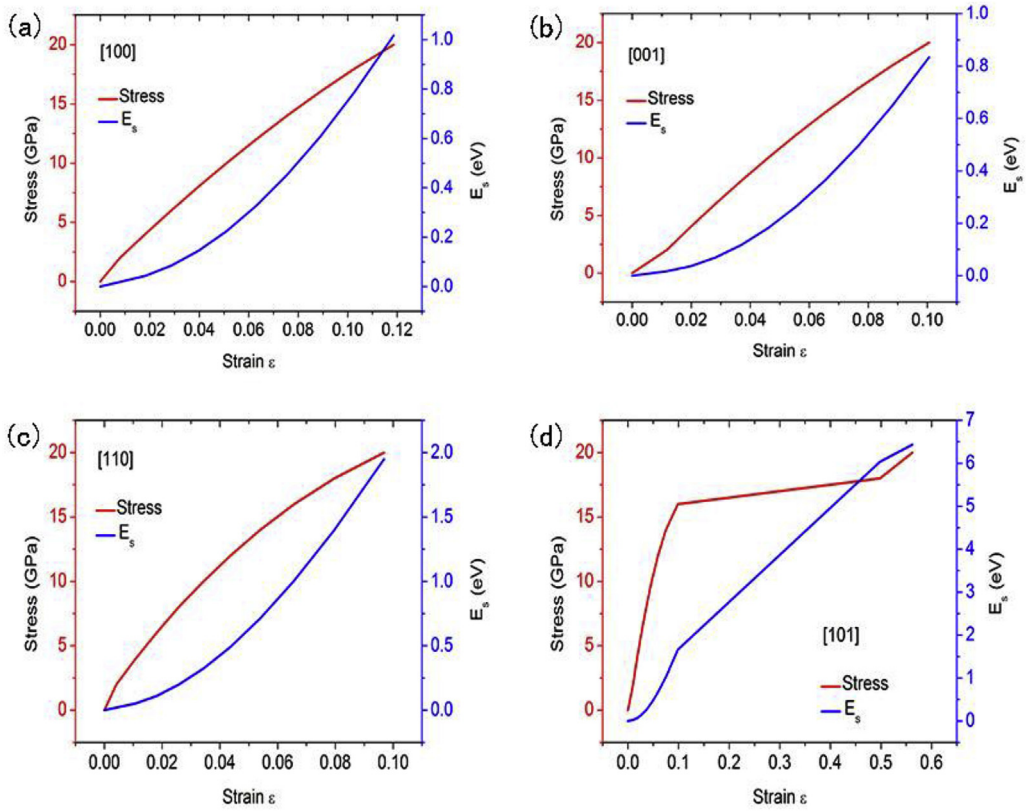

Fig. 1. The strain energy VS strain and stress VS strain along the (a) [100], (b) [001], (c) [110], and (d) [101] crystallographic directions.

2. Computational details

In this research, the calculations were performed by the first-principles density functional theory (DFT) within the CASTEP (Cambridge Serial Total Energy Package) code [22,23]. The ultrasoft pseudo-potential and the generalized gradient approximation (GGA) with the WC formula were used to describe the electron-core interaction and exchange-correlation potentials [24,25], respectively. All calculations for $NbAl_3$ were performed with the plane-wave cutoff energy of 400 eV and the Monkhorst-Pack mesh [26] ($4 \times 4 \times 2$). The valence electron configurations for two elements were Nb $4s^2 4p^6 4d^4 5s^1$ and Al $3s^2 3p^1$, respectively. The thresholds for energy change per atom, maximum force, maximum stress and maximum displacement for the converged structures ensured the convergences of 5×10^{-6} eV/atom, 0.01 eV/Å, 0.02 GPa and 5×10^{-4} Å. To study the physical properties under different tension conditions, the different tensions along the [100], [001], [110], and [101] directions were set in the CASTEP code.

3. Results and discussion

3.1. Mechanical properties under zero tension

The calculated lattice parameters of $NbAl_3$ are $a = 3.8458$ Å and $c = 8.6094$ Å, which are in good agreement with the experimental data [1,6,16,19]. The elastic constants (C_{ij}), bulk modulus (B), shear modulus (G), Young's modulus (E), Poisson's ratio (ν), Pugh's criterion (B/G) and Cauchy's pressure (C_{12}-C_{44}) of tetragonal $NbAl_3$ are calculated under zero tension, which are shown in Table 1. We can see that the mechanical parameters all agree well with previous data [8,11,12], meaning that our computational work is highly reliable. Owing to the symmetry of 4/mmm Laue group, it is six independent elastic constants for tetragonal $NbAl_3$. The elastic constant C_{11} is less than C_{33}, indicating that the a-axis anti-deformation ability is weaker than the c-axis anti-deformation ability. The $C_{66} > C_{44}$ shows that the shear deformation resistance of (001) is stronger than that of (100). The corresponding stability criterion for tetragonal structure are: $C_{11} > |C_{12}|$, $2C_{13}^2 < C_{33}(C_{11} + C_{12})$, $C_{44} > 0$,