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Ab Initio Study of Structural, Elastic, Electronic Properties of Antiperovskite $AlCTi_3$, AlC_2Ti_3 and Al_2CNiTi_3

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Abstract

We investigate the Structural, elastic and electronic proprieties of the intermetallic antiperovskite $AlCTi_3$, AlC_2Ti_3 and Al_2CNiTi_3 using the first principal. The calculations are based on the plane wave pseudo potential method (PP-PW) with the generalized gradient approximation (GGa). Lattice parameters were found to be agreement with available experimental results. In the pressure range that we have employed, mechanical stability criteria were verified instead for values of applied pressures up 40 GPa, elastic moduli were calculated and the mechanical stability criteria were verified. By analysing the B/G ratios for $AlCTi_3$, AlC_2Ti_3 and Al_2CNiTi_3 compounds, it is found that are brittle nature and we observed that Al_2CNiTi_3 when compared with other could be less brittle than other compounds and should have the highest conductivity. The band structure of these compounds has been found to display a metallic character and reveal that are conductor. The covalent ionic band nature is due to the strange hybridization between Ti and C atoms. We have observed based on the overlap population analysis that the values being related to the bonding states. We noticed that the C-Ti bonds increase when the carbon is doubled in AlC_2Ti_3 further strengthens the above fact that AlC_2Ti_3 could be more brittle.

Keywords: Perovskite, Gg A, Electronic Structure, Elastic Moduli.

Introduction

In the past decade, antiperovskite have attracted significant attention of the researchers, for having utility in different industrial applications, The antiperovskite compounds with the formula AXM3, in which X is a principal element pertaining to group (III-V), A being carbon, nitrogenizes or boron and M are a metal of transition [1]. There are several phases in the Ti–Al–C ternary compounds system, which includes Ti_3AlC. The unique combination of ceramics and metallic properties give more attention to this system [2, 3].

$AlCTi_3$ attract a lot attention from researchers who have studied their physical properties, using different methods [4]. They show that is a metallic material, and that the strong hybridization between Ti-3d and Al-3p states stabilizes the structure [5]. Others propose that when there is an increase in the anti-bonding state between Ti and Al atoms, the stiffness decreases [5, 6].

The present study is to focus mainly on the Ti-based alumino carbide with the anti-perovskite structure and influence of Nickel when it was introduced, which is less explored both experimentally and theoretically, in order to know the properties structural, elastic and electronic of Ti_3AlC, AlC_2Ti_3 and Al_2CNiTi_3 to determine them for technological advantages. The remainder of the paper is organized as follows. In Sec. II, we describe of our first principles calculations. In Sec. III, we report the results of our simulations (the structural, elastic and electronic properties). Finally, the main conclusions of this work reviewed in Sec. IV.

Calculation Methods

$AlCTi_3$, AlC_2Ti_3 and Al_2CNiTi_3 antiperovskite materials have a cubic structure, for $AlCTi_3$ and Al_2CNiTi_3 (space group Pm3m and Fd-3ms respectively) and hexagonal structure for AlC_2Ti_3 (space group P63/mmc), with experimental lattice parameters of a_{AlCTi3} = 4.156A°, $a_{AlC2Ti3}$ = 3.073A°; $b_{AlC2Ti3}$=18.557A°and $a_{Al2CNiTi3}$=11.463A° (See Table 1). In this paper, we studied the surfaces of $AlCTi_3$, AlC_2Ti_3 and Al_2CNiTi_3 using Density Functional Theory (DFT) with plane wave (PW) basis set (DFT-PW method). The first-principles ab-initio method have already used to check how sensitive surface relaxation proprieties, for describing the valence bands. The following basis set Ti(3s, 3p, 4s, 3d), C(2s, 2p), Al(3s, 3p) of $AlCTi_3$, Ti($3s^2$,$3p^6$,$3d^2$,$4s^2$) ,C($2s^2$,$2p^2$), Al($3s^2$,$3p^1$) of AlC_2Ti_3 and Ti($3s^2$,$3p^6$,$3d^2$,$4s^2$),C($2s^2$,$2p^2$),Al($3s^2$,$3p^1$),Ni($3d^8$,$4s^2$) of Al_2CNiTi_3 are used in the calculations. The exchange–correlation potential is treated with the generalized gradient approximation (GGA) of [7]. It is taking into account the gradient of the density at the same coordinate.

In order to perform first-principles and DFT calculation we used the CASTEP (Cambridge Serial Total Energy Package computer code [8]. This code explores the properties of crystals and surfaces in materials such as semiconductors, ceramics, metals, minerals, and zeolites. We have set the energy cut off for the plane wave expansion at 380 eV, which was large enough to obtain good convergence. In the Brillouin zone integrations, the k point at 6 ×6 ×6, 9×9×2 and 1×1×1and were determined according to Monkhorst_Pack scheme [9].

For $AlCTi_3$, AlC_2Ti_3 and Al_2CNiTi_3, respectively. In our calculation we are not using spin polarized, because the result of the energy difference $\Delta E= E^{SP} – E^{SG}$ ›0. These results correspond to the fact that the ferromagnetic phase is more stabilized than antiferromagnetic phase and vice versa.

Table 1: Calculated a_0 (in Å), B_0 (in GPa), V (A**³) and B' (calculated from Birch_Murnaghan EOS fitting); A; G; E; µ; ʎ; σ and B/G and elastic constants C_{ij}.

Compounds	$AlCTi_3$	AlC_2Ti_3	Al_2CNiTi_3
Phase	Pm3m	P63/mmc	Fd-3ms
a(A)°=b	4.151(4.156) a	3.057(3.073) b	8.047(11.463) c
C(A)°	-	18.555(18.557) d	
V(A3)	71.532	150.25	368.58
B0(Gpa)	157.65	164.77	158.67
B'(GPa)	3.58	3.71	4.2
G (GPa)	109.24	135.49	122.293
Ex,y(GPa)	315.79	347.28	254.516
Ez (GPa)	-	279.10	-
µx,y	59.35	144.65	103.58
µz	-	120.18	-
ʎ	84.82	74.44	83.80
σx,y	0.166	0.2004	0.232
σz	-	0.161	-
A	0.693	0.955	1.150
B/G	1.44	1.21	1.41
C11	338.18	374.001	296.322
C12	67.387	75.227	89.843
C44	94.607	127.038	118.770
C13	-	72.348	-
C33	-	302.403	-

Results and Discussion

Structural Proprieties and Elastic Properties

In first places, we calculate the lattice constants a (Å) for the antiperovskite $AlCTi_3$, AlC_2Ti_3 and Al_2CNiTi_3 which are shown in table1. The results that we obtained was closer to the measured experimental ones, with a small difference due to the reliability of present first-principal calculations with the generalized gradient approximation GGA (WC) [10]. The bulk modulus B at zero pressure and its pressure derivative B_0 are calculated by fitting pressure_ volume data to a third-order Birch_ Murnaghan equation of state (EOS), employing a dense sampling technology in the low-pressure region [11]. Hence our results for B are good and accurate (Fig. 1). To build up the (P_V) EOS for $AlCTi_3$, AlC_2Ti_3 and Al_2CNiTi_3 for pressure values up to 40GPa (Fig.1), from which we have extracted the values of the bulk modulus and its pressures derivative, see table 1, it can observe that B growth by 4.5% when going from $AlCTi_3$ to AlC_2Ti_3 and by 0.6% when going from $AlCTi_3$ to Al_2CNiTi_3. Our calculated values of the pressure derivative B' increase slightly from 3.58 for $AlCTi_3$ to 4.2 for Al_2CNiTi_3.

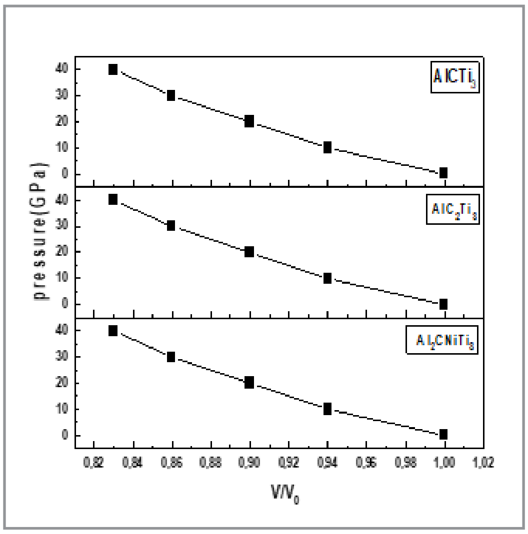


Figure 1: Pressure-Volume Dependence for $AlCTi_3$, AlC_2Ti_3 and Al_2CNiTi_3 Compounds

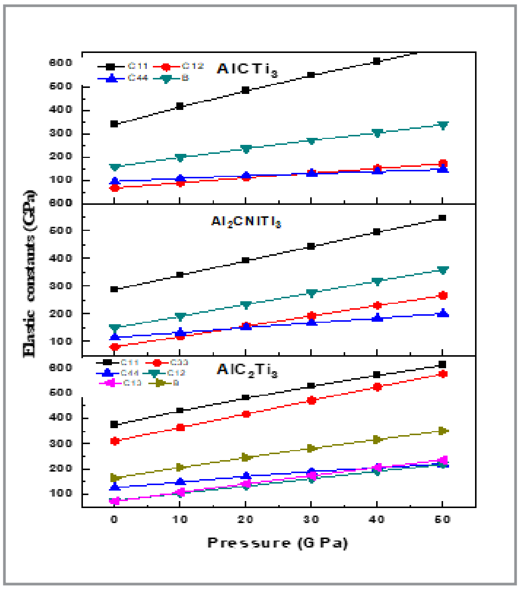


Figure 2: Pressure- Elastic Constants Dependence for $AlCTi_3$, AlC_2Ti_3 and Al_2CNiTi_3

The elastic constants of AlCTi3, AlC2Ti3 and Al2CNiTi3 compounds are listed in Table 1. The errors quoted for Cij values are associated with the deviation of the stress strain relationship from linearity [10]. There are 21 independent elastic constants, Cij, but the symmetry of the cubic crystal lattice reduces this number to only three independent elastic constants C11, C12, and C44. And five elastic constants of hexagonal crystal. The bulk modulus B of cubic system can be expressed as a linear combination of C11 and C12:

$$B=(C11+2C12)/3. \quad (1)$$

And of Hexagonal System:

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

$$B_V=\frac{2}{9}\left[C_{11}+C_{12}+2C_{13}+\frac{1}{2}C_{33}\right] \quad (3)$$

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

Crystals are directly related to the anisotropy of thermal and elastic properties [12]. We calculated the anisotropy factor A (Table 1) of our compounds by using the following expression for cubic symmetry:

$$A=\frac{2C_{44}}{C_{11}-C_{12}} \quad (5)$$

And for hexagonal symmetry:

$$A=\frac{4C_{44}}{C_{11}+C_{33}-2C_{13}} \quad (6)$$

With the respect to the variation of pressure, we present the variation of the elastic constants and the bulk modulus B of AlCTi3, AlC2Ti3 and Al2CNiTi3 compounds In Fig.2.

Poisson's ratio σ, the Lame coefficients λ, μ and the Young's modulus E, are frequently measured for polycrystalline materials characterizing their hardness [11, 12].

These Quantities Are Given by the Following Equations [13].

$$\frac{9BG}{3B+G} \quad (7)$$

$$\lambda=\frac{E\sigma}{1-\sigma-2\sigma^2} \quad (8)$$

$$\mu=\frac{E}{2+2\sigma} \quad (9)$$

$$\sigma=\frac{3B-E}{6B} \quad (10)$$

The calculated and the deduced values of B, G, E, σ, λ and μ for AlCTi3, AlC2Ti3 and Al2CNiTi3 crystal are listed in Table 1.

There are no exact expressions for poly-crystal averaged shear moduli in terms of the Cij, but one can evaluate approximate averages of the lower and upper bounds given by various theories. According to Hill, the arithmetic average of the Voigt and Reuss values can be used to estimate the average shear modulus which is represented as GH and is shown in the following relations [14 -16].

$$GH=\frac{G_R+G_V}{2} \tag{11}$$

For a cubic crystal:

$$GV=\frac{3C_{44}+C_{11}+C_{12}}{5} \tag{12}$$

$$GR=\frac{5(C_{11}-C_{12})C_{44}}{4C_{44}+3(C_{11}-C_{12})} \tag{13}$$

And For a hexagonal crystal:

$$GV=\frac{1}{30}[7C_{11}-5C_{12}-4C_{13}+2C_{33}+12C_{44}] \tag{14}$$

$$GR=\frac{5}{2}\left\{\frac{[(C_{11}+C_{12})C_{33}-2C_{13}^2]C_{44}C_{66}}{3B_V C_{44}C_{66}+[(C_{11}+C_{12})C_{33}2C_{13}^2](C_{44}+C_{66})}\right\} \tag{15}$$

To explain further the ductile or brittle nature of the compounds. We discussed the B/G ratio, if B/G>1.75, the material is expected to be ductile. Otherwise, the material behaves in brittle, according to Pugh's empirical relationship [17]. In our case the value of B/G<1.75 for all compounds, be classified as brittle materials (see table 1).

The hardness of a material is defined as its resistance to deformation and fracture. We notice that shear modulus G (represent the resistance to plastic deformation) and bulk modulus B (represent the resistance to fracture) gradually increases with phase change (cubic → hexagonal). Young's modulus of Al_2CNiTi_3 is found to be 254.516 GPa, which is quite lower when compared to Young's modulus value of $AlCTi_3$ (315.79GPa) and AlC_2Ti_3 (347.28GPa), respectively. In general, the covalent nature of the compound increases when Young's modulus increases, which further has an impact on the ductility of the compounds. This result can be explained when nickel was introduced.

We try to explain more calculated study, the Poisson's ratio generally quantifies the stability of the crystal. Here the value of σ is around 0.166 for AlCTi3 and 0.232 for Al_2CNiTi_3, the increase in the value when going from AlCTi3 to Al_2CNiTi_3 clearly shows that the ductility should be higher in Al_2CNiTi_3.

From (Fig.2), it appears that AlC2Ti3 possesses the highest elastic moduli among the studied compounds. On the other hand, concerning the stability of materials elastic moduli have great importance [11]. All Cij constants are positive and satisfy the criteria for these compounds [18].

We observe in all the curves of the three compounds in the pressure range considered a linear dependence. C11 is more sensitive to pressure change than other elastic modules. C44 is the least sensitive to pressure change. For a cubic crystal to be mechanically stable, it must obey the following conditions:

$$C_{44}-P>0 \tag{16}$$

$$(C_{11}-C_{12})/2-p>0 \tag{17}$$

$$(C_{11}+2C_{12}+P)/3>0. \tag{18}$$

For a hexagonal crystal, the conditions of mechanical stability are as follows:

$$C_{11}>0\ ;\quad C_{33}>0\ ;\quad C_{44}>0\ ;\quad C_{66}>0 \tag{19}$$

$$C_{11}-C_{12}>0\ ;\quad (C_{11}+C_{12})C_{33}>2C_{13}^2 \tag{20}$$

$$C_{11}+C_{12}+C_{33}>0 \tag{21}$$

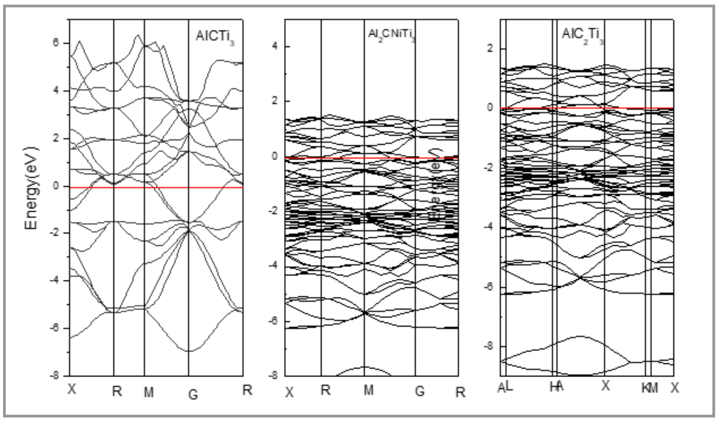
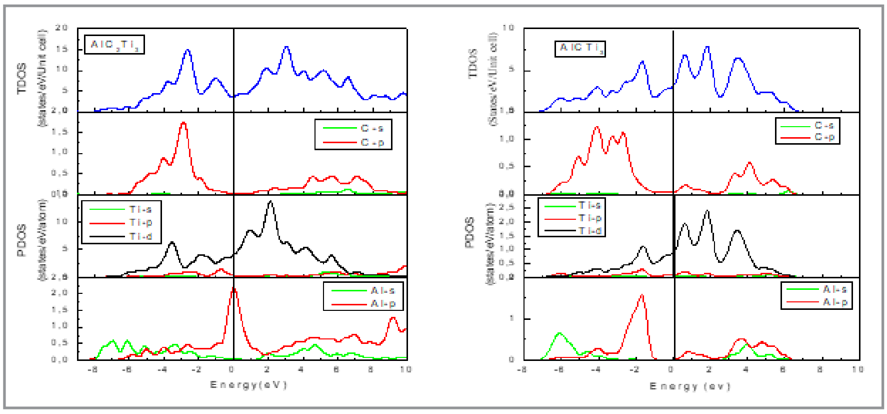


Figure 3: Calculated Band Structures for $AlCTi_3$, AlC_2Ti_3 and Al_2CNiTi_3, Fermi level is set at 0 eV.



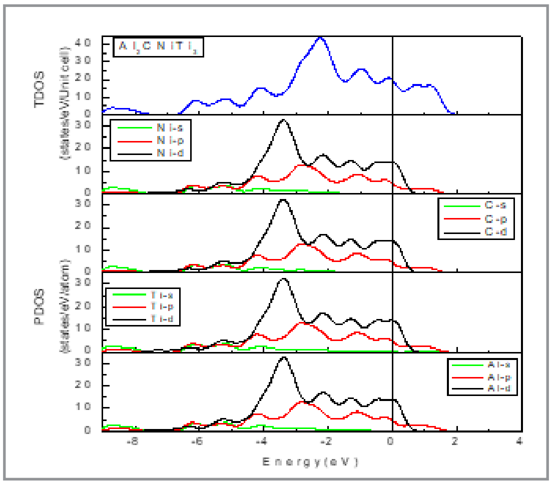


Figure 4: Total And Partial Density of States for AlCTi3, AlC2Ti3and Al2CNiTi3, Vertical Dashed Lines Denote the Fermi Level

The band structure,total(TDOS),atomic site projected densities of states (PDOS) and bonding charge density of these compounds, which have been calculated for the equilibrium geometry of our compounds, are shown in Figs. 4. Energy band structure of $AlCTi_3$, $AlC_2Ti_3$and Al_2CNiTi_3 compounds along the high symmetry Point in the Brillouin zone as illustred in Fig.3. The non existence of a gap at Fermi level confirms the metallic character of all the compounds under study and indicates the respective presence of conducting features. Since the electrical conductivity is related to the empty states, and based on the total and partial density of states (TDOS and PDOS), from fig.4, with a TDOS at the fermi level equal to 17.53 it can be expected that $AlCNiTi_3$ have the highest conductivity; and with a value of TDOS equal to 3.10 States/eV/Unitcell [19]. $AlCTi_3$ have the lowest conductivity .On the other side. for $AlCTi_3$ and AlC_2Ti_3 the origin of the band structure spectra is due to C_p,Ti_d,Al_s and Al_p states in the energy range of -8 to -1.5 eV. From -1.5 to fermi level, the band structure is originally derived from the Ti_d states. The main part of the conductivity is assured by the d electrons of the transition metal Ti, beyond the Fermi level, Ti_d states remain majority, with little contribution of Al_p states.

Table 2: Overlap Population for Nearest Neighbours in $AlCTi_3$, AlC_2Ti_3 and Al_2CNiTi_3

Compounds	$AlCTi_3$	AlC_2Ti_3	Al_2CNiTi_3
Bond population	C-Ti Ti-Al	C-Ti	C-Ti Al-Ni Ti-Al Ti-Ni
	0.63 0.86	1.16 0.88	0.41 0.34 0.32 0.21

We calculated the overlap population of the nearest neighbours in the crystal (Table2), in order to analyse the binding properties. The values being related to the bonding states [20, 21]. This correlates with the relatively high value of the mass modulus of this compound. We noticed that the C-Ti bonds increase when the carbon is doubled in AlC_2Ti_3.

Conclusion

In summary, the structural, elastic and electronic properties of $AlCTi_3$, AlC_2Ti_3 and AlC_2Ti_3 compounds have been calculated using (PP-PW) approach based on density functional theory, with in the generalized gradient approximation (GGA). Equilibrium volumes and Lattice parameters were calculated and show with the available experimental data a good agreement. The values of the B/G ratios for $AlCTi_3$, AlC_2Ti_3 and AlC_2Ti_3 compounds show that are brittle nature. The high Poisson's ratio associated with AlC_2Ti_3 when compared with other compounds arrive at the solution that AlC_2Ti_3 could be less brittle. It is appeared that AlC_2Ti_3 possesses the highest elastic constants.

In addition, we have observed that the values being related to the bonding states based on the overlap population analysis. We noticed that the C-Ti bonds increase when the carbon is doubled in AlC_2Ti_3 further strengthens the above fact that AlC_2Ti_3 could be more brittle. The GGA band structure calculations show that our compounds are strong conductors, expected that AlC_2Ti_3 should have the highest conductivity. Finally, we hope that these predictions will be useful for further experimental works on these unexplored compounds.

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References

1. Cherrad, D., Selmani, L., & Maouche, D. (2011). First principles calculations on elasticity, electronic structure and bonding properties of antiperovskites $ANTi_3$ (A = Al, In and Tl). Journal of Alloys and Compounds, 509, 4357–4362.
2. Schuster, J. C., Nowotny, H., & Vaccaro, C. (1980). The ternary systems Cr–Al–C, V–Al–C, and Ti–Al–C and behavior of H-phases (M_2AlC). Journal of Solid-State Chemistry, 32, 213–219.
3. Wilhelmsson, O., Palmquist, J. P., Lewin, E., Emmerlich, J., Eklund, P., Persson, P. O. A., Högberg, H., Li, S., Ahuja, R., Eriksson, O., Hultman, L., & Jansson, U. (2006). Deposition and characterization of ternary thin films within the Ti–Al–C system by DC magnetron sputtering. Journal of Crystal Growth, 291, 290–300.
4. Medkour, Y., Roumili, A., & Boudissa, M. (2009). Struc-

tural, elastic and electronic properties of ACTi₃ (A = Al, In and Tl) antiperovskite. Solid State Communications, 149, 919–922.

5. Zhang, X., Wang, X., Fangzhi, L., & Zhou, Y. (2009). Mechanical and thermal properties of antiperovskite Ti_3AlC prepared by an in-situ reaction/hot-pressing route. Journal of the American Ceramic Society, 92(11), 2698–2703.
6. Kanchana, V. (2009). Mechanical properties of Ti_3AlX (X = C, N): Ab initio study. EPL (Europhysics Letters), 87, 26006.
7. Perdew, J. P., Burke, K., & Ernzerhof, M. (1996). Generalized gradient approximation made simple. Physical Review Letters, 77, 3865–3868.
8. Segall, M. D., Lindan, P. J. D., Probert, M. J., Pickard, C. J., Hasnip, P. J., Clark, S. J., & Payne, M. C. (2002). First-principles simulation: Ideas, illustrations and the CASTEP code. Journal of Physics: Condensed Matter, 14, 2717–2744.
9. Monkhorst, H. J., & Pack, J. D. (1976). Special points for Brillouin-zone integrations. Physical Review B, 13, 5188–5192.
10. Nowotny, V. H. (1970). Progress in solid state chemistry. Progress in Solid State Chemistry, 2, 27–58.
11. Debard, Y. (2011). Mécanique, thermique et éléments finis (Mars 2006). 31.
12. Green, D. J. (1998). An introduction to the mechanical properties of ceramics. Cambridge University Press.
13. He, Y., Schwarz, R. B., Migliori, A., & Whang, S. H. (1995). Elastic constants of single crystal γ-TiAl. Journal of Materials Research, 10, 1187–1195.
14. Hill, R. (1952). The elastic behaviour of a crystalline aggregate. Proceedings of the Physical Society, 65, 350–354.
15. Voigt, W. (1889). On the relation between the elasticity constants of isotropic bodies. Annalen der Physik und Chemie, 38, 573–587.
16. Reuss, A. (1929). Calculation of the yield point of polycrystalline materials. Zeitschrift für Angewandte Mathematik und Physik, 9, 49–58.
17. Pugh, S. F. (1954). Relations between the elastic moduli and the plastic properties of polycrystalline pure metals. The London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science, 45, 823–843.
18. Wang, J., Yip, S., Phillpot, S. R., & Wolf, D. (1993). Crystal instabilities at finite strain. Physical Review Letters, 71, 4182–4185.
19. Ashcroft, N. W., & Mermin, N. D. (1976). Solid state physics. Saunders College.
20. Segall, M. D., Pickard, C. J., Shah, R., & Payne, M. C. (1996). Population analysis in plane wave electronic structure calculations. Molecular Physics, 89, 571–577.
21. Segall, M. D., Shah, R., Pickard, C. J., & Payne, M. C. (1996). Population analysis of plane-wave electronic structure calculations of bulk materials. Physical Review B, 54, 16317–16320.

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