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Pressure Dependence of Structural, Elastic and Electronic Properties of α-Al_2O_3: First-principles Calculations

(Tekanan Pergantungan kepada Sifat Struktur, Anjal dan Elektronik α -Al_2O_3: Pengiraan Prinsip-Pertama)

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ABSTRACT

The first-principles calculations were performed to investigate the structural, elastic, mechanical and electronic properties of α-Al_2O_3 at applied pressure up to 50 GPa. The obtained ground state properties were in agreement with previous experimental and theoretical data. The elastic constants, bulk modulus, shear modulus, Young's modulus and anisotropy have been calculated as pressure increased. It was found that there was a brittle-ductile transition at about 23.2 GPa. The increasing ratio B_a/B_c with pressure indicates the weakening chemical bonding and the increasing anisotropy in this compound. The electronic structures were also calculated, which shows that band gaps increase monotonically. The population analysis showed the charge transfer was mainly between Al-3s and O-2p as pressure increased.

Keywords: Density functional theory; elastic properties; electronic structure; α-Al_2O_3

ABSTRAK

Pengiraan prinsip-pertama dijalankan untuk mengkaji sifat struktur, anjal, mekanik dan elektronik α-Al_2O_3 pada tekanan yang dikenakan sehingga 50 GPa. Sifat keadaan tanah yang diperoleh adalah sama dengan data uji kaji dan teori yang terdahulu. Pemalar anjal, modulus pukal, modulus ricih, modulus Young dan anisotrofi telah dihitung apabila tekanan meningkat. Didapati bahawa terdapat peralihan rapuh-mulur pada 23.2 GPa. Peningkatan nisbah B_a/B_c dengan tekanan menunjukkan ikatan kimia yang semakin lemah dan anisotrofi yang semakin meningkat dalam sebatian ini. Struktur elektronik juga dihitung yang menunjukkan bahawa jurang jalur meningkat secara senada. Analisis penduduk menunjukkan pemindahan caj antara Al-3s dan O-2p apabila tekanan meningkat.

Kata kunci: Sifat anjal; struktur elektronik; teori fungsi ketumpatan; α-Al_2O_3

INTRODUCTION

Al_2O_3 is an extremely important ceramic material to industrial applications (Chen et al. 2008; Kruse et al. 1996; Matsunaga et al. 2003; Zhukovskii et al. 2001). The many applications alumina are its use as a coating for cemented carbide cutting tools, high-$\varkappa$ gate dielectrics, multilayer structures with high damage thresholds in UV laser applications, heterogeneous catalysis, corrosion protection and thermal barriers coating (Ahuja et al. 2004; Copel et al. 2001; Fernández et al. 2003[a], 2003b; Gusev et al. 2001; Haverty et al. 2002; Hosseini et al. 2005a, 2005b; Liao et al. 1999; Ollivier et al. 1997; Shang et al. 2007; Shi et al. 2006; Vali & Hosseini 2004; Yang et al. 2009, 2004) due to its high band gap and band offset properties, high dielectric constant, high hardness, high mechanical strength, good abrasion resistance, good corrosion resistance and good electrical insulation.

Among those applications, Al_2O_3 as a thermal barrier coating has been paid much attention (Limarga et al. 2005, 2002; Shanmugavelayutham et al. 2006; Widjaja et al. 2002; Yu et al. 2010). This application is needed to measure and monitor the change of stress in the thermally grown oxide layer to understand the oxidation resistance, where the elastic properties that show the response to an applied macroscopic stress are required to study. On the other hand, the basic thermodynamic variable of pressure is used to transport matter and develop the micromechanical devices. Moreover, as a promising gate dielectric material in metal-oxide-semiconductor (MOS) devices, it is important to study the pressure dependence of the band gaps because the electronic properties of strained lattices can be obtained by investigating the effects of strain on bulk samples.

Theoretically, there are many works to study Al_2O_3, e.g. the first-principles plane-wave pseudopotential calculations with VASP code (Matsunaga et al. 2003), the full potential-linearized augmented plane wave method with WIEN2k package (Hosseini et al. 2005b), the first-principles pseudopotentials and plane waves with ABINIT code (Vali & Hosseini 2004), the first-principles density functional calculations with SIESTA code (Fernández et al. 2003b) and the full-potential linear muffin-tin-orbital (FPLMTO) method (Ahuja et al. 2004). However, the application of pressure on Al_2O_3 to study the pressure dependence of the structural, elastic and electronic properties was not taken into account. Therefore, the investigation Al_2O_3 under pressure is essential.

In this paper, we show the first-principles calculations to investigate the properties of α-Al_2O_3 under pressure.

The calculational methods are shown in the next section, the results and discussion are presented next and the conclusions are given in the last section.

Computational Methods

Total Energy and Geometry Optimization Calculations

The calculations are performed using the plane-wave ultrasoft pseudopotential with the generalized gradient approximation (GGA) as parameterized by Perdew et al. (1992) with CASTEP code (Segall et al. 2002). The kinetic energy cutoff of 380 eV and the k-point meshes of 6×6×6 for α-Al_2O_3 have been set to structure optimization and energy calculation. The Al $3s^2, 3p^1$, O $2s^2, 2p^4$ electrons are explicitly treated as valence electrons. The convergence criterion for the maximal force between atoms is 0.01 eV/Å, the maximum stress is 0.02 GPa and the maximum displacement is 5.0×10^{-4}Å.

Elastic Properties

The elastic constants are important parameters that describe the response to an applied macroscopic stress, which are defined by means of a Taylor expansion of the total energy $E(V, \delta)$ for a strained system of volume V with respect to a strain parameter δ (Chen 1996; Fast et al. 1995; Tian 2004). As a matter of fact, the structure of α-Al_2O_3 has six independent elastic constants c_{11}, c_{12}, c_{13}, c_{14}, c_{33} and c_{44}. The mechanical stability conditions for α-Al_2O_3 under pressure are known as (Sin'ko & Smirnov 2002):

$$\tilde{c}_{44} > 0, \tilde{c}_{11} > |\tilde{c}_{12}|, \ \tilde{c}_{33}(\tilde{c}_{11} + \tilde{c}_{12}) > 2\tilde{c}_{13}^2, \tag{1}$$

where $\tilde{c}\alpha\alpha = c_{\alpha\alpha} - P(\alpha=1, 3, 4), \tilde{c}_{12} = c_{12} + P, \tilde{c}_{13} = c_{13} + P$.

The Voigt approximation has proposed the averaging of relations expressing the stress in terms of the given strain (Voigt 1928) and the Reuss approximation has proposed the averaging of the relations expressing the strain in terms of the given stress (Reuss 1929). Hill (1952) has proved that the Voigt and Reuss equations represent upper and lower bounds of elastic constants, respectively. Hence, he took an arithmetic mean value of the two approaches as follows:

$$B_{Hill} = \frac{1}{2}(B_{Reuss} + B_{Voigt}) = \frac{1}{2}\left\{\left[(2s_{11}+s_{33})+2(s_{12}+2s_{13})\right]^{-1} + \left[\frac{1}{9}(2c_{11}+c_{33})+\frac{2}{9}(c_{12}+2c_{13})\right]\right\}. \tag{2}$$

$$G_{Hill} = \frac{1}{2}\left(G_{Reuss} + G_{Voigt}\right) = \frac{1}{2}\left\{15\left[4\left(2s_{11}+s_{33}\right)-4\left(s_{12}+2s_{13}\right)+6\left(s_{44}+s_{11}-s_{12}\right)\right]^{-1} + \left[\frac{1}{15}\left(2c_{11}+c_{33}-c_{12}-2c_{13}\right)+\frac{1}{5}\left(2c_{44}+\frac{c_{11}-c_{12}}{2}\right)\right]\right\}, \tag{3}$$

where s_{ij} is the inverse matrix of the elastic constants matrix c_{ij}.

Then, the Young's modulus E is calculated using (4):

$$E = \frac{9BG}{G+3B}, \tag{4}$$

Results and Discussion

Structural Properties

α-Al_2O_3 is a trigonal crystal system with space group $R\bar{3}c$ and local symmetry D_{3d}^6. In order to determine the equilibrium geometry, we first calculate the structural properties using the obtained total energy as a function of volume and the third-order Birch-Murnaghan equation of state (Murnaghan 1944). The calculated results are summarized in Table 1 together with previous available theoretical (Duan et al. 1999, 1998; Matsunaga et al. 2003; Shang et al. 2007; Ru & Qiu 2009) and experimental (d'Amour et al. 1978; Lee & Lagerlof 1985) data. Obviously, we can see that our results are in agreement with the experiments and calculations. Figure 1 displays the pressure dependence of the normalized structural parameters a/a_0, α/α_0 and V/V_0 from 0 to 50 GPa (a_0, α_0 and V_0 are experimental data). As pressure increasing, the a/a_0 and V/V_0 decrease whereas α/α_0 increases. The best fit of these curves show an almost linear behavior presented in Figure 1.

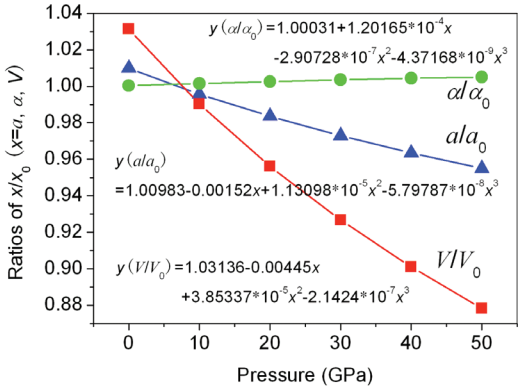

FIGURE 1. The pressure dependence of the normalized structural parameters a/a_0, α/α_0 and V/V_0 from 0 to 50 GPa

Elastic Properties

Elastic constants are important parameters of materials, give worth information to study the structural stability, determine the response of the crystal to external forces and provide a link between the mechanical and dynamical behaviors of crystals. The calculated six independent elastic constants are listed in Table 1 together with the available experimental (Gieske & Barsch 1968; Gladden et al. 2004; Hovis et al. 2006) and theoretical (Duan et

TABLE 1. Calculated lattice parameters a (Å), α (°), volume V_0 (Å^3), elastic constants c_{ij} (GPa), bulk modulus B, B_a, B_c (GPa), shear modulus G (GPa), Young's modulus E, E_x, E_z (GPa), bulk modulus to shear modulus ratio (B/G) of α-Al_2O_3 at 0 GPa and 0 K

	This work	Other theoretical data	Expt.
a	5.1785	5.195[a], 5.111[b], 5.180[c], 5.096[d], 5.107[e]	5.136[h], 5.128[i]
α	55.2961	55.32[a], 55.37[b], 55.30[c], 55.36[d], 55.41[e]	55.286[h], 55.28[i]
V_0	87.4624	87.5[c], 83.5[d]	84.8[i]
c_{11}, c_{12}, c_{13}, c_{14}, c_{33}, c_{44}	447.5, 145.9, 102.0, 0, 453.1, 128.0	451.5[c], 148.4[c], 107.6[c], 20.2[c], 454.9[c], 131.7[c], 497.1[d], 164.7[d], 129.5[d], 18.6[d], 492.5[d], 154.2[d], 485.755[f], 165.988[f], 125.422[f], 0[f], 484.657[f], 143.491[f], 502[g], 161[g], 125[g], -19[g], 501[g], 157[g]	498[j], 163[j], 117[j], -23[j], 502[j], 147[j], 497[k], 163[k], 116[k], 22[k], 501[k], 147[k]
B	227.4	231.7[c], 259.3[d], 258[g]	255[j], 254[k]
B_a	706.5		
B_c	637.1		
G	146.7	149.3[c], 165.8[d], 168[g]	163[j], 165[k]
E	362.1		
E_x	388.9		
E_z	418.1		
B/G	1.551		

[a] GGA (Matsunaga et al. 2003), [b] LDA (Matsunaga et al. 2003), [c] GGA (Shang et al. 2007), [d] LDA (Shang et al. 2007), [e] (Duan et al. 1998), [f] (Ru & Qiu 2009), [g] (Duan et al. 1999), [h] (d'Amour et al. 1978), [i] (Lee & Lagerlof 1985), [j] (Gieske & Barsch 1968) and [k] (Gladden et al. 2004; Hovis et al. 2006)

al. 1999; Ru & Qiu 2009; Shang et al. 2007) data at 0 GPa and 0 K. According to the Born stability conditions at 0 GPa for trigonal structures ($C_{44} > 0$, $C_{11} > |C_{12}|$, $C_{33}(C_{11} + C_{12}) > 2C_{13}^2$ (Born & Huang 1982)), our calculated results satisfy these criteria, which indicates α-Al_2O_3 was mechanically stable. We also calculate the bulk modulus, shear modulus, Young's modulus, Young's modulus along the x- and z-axis, B/G using (2)-(4), which are given in Table 1. We can see that our results are consistent with previous theoretical (Duan et al. 1999; Shang et al. 2007) and experimental (Gieske & Barsch 1968; Gladden et al. 2004; Hovis et al. 2006) data. The parameter limiting the stability of this compound is shear modulus due to $B>G$. As we know, the bulk modulus represents the resistance to fracture and the shear modulus represents the resistance to plastic deformation. A material is ductile (brittle) if the B/G is more (less) than 1.75 (Pugh 1954). In this case, this compound is described as brittle. The mechanical anisotropy is computed by using the bulk moduli B_a and B_c (shown in Ref. (Ravindran et al. 1998; Zhu et al. 2008)) along the a- and c-axis, respectively. The ratio B_a/B_c is 1.109 which indicates this compound has strong chemical bonding and anisotropy.

Elastic properties under pressure are studied in detail. The pressure dependence of elastic constants is shown in Figure 2, which shows the elastic constants increase almost linearly with increasing pressure. The calculated elastic constants are fitted to quadratic functions shown in Figure 2 and the first- and second-order pressure derivatives are also presented. The calculated results satisfied the Sin'ko's and Smirnov's conditions of mechanical stability shown in (1) under pressure up to 50 GPa. Figure 3 shows the pressure dependence of bulk modulus, shear modulus, Young's modulus, E_x, E_z, B_a, B_c and B/G. We can see that these parameters increase with increasing pressure, but with different slopes. The B/G varies rapidly and shows the change from brittle property to ductile property as pressure increases. The change pressure is about 23.2 GPa. The slopes of B_a and B_c are moderate. The increasing ratio

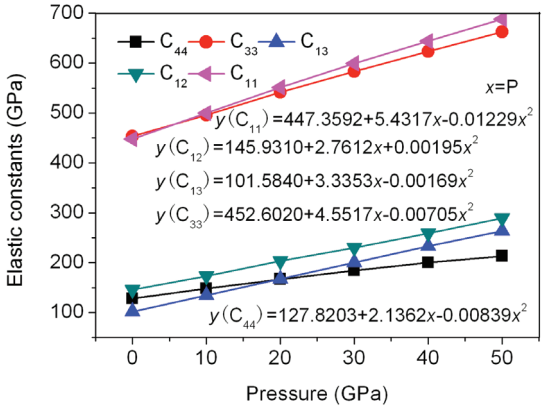

FIGURE 2. The pressure dependence of elastic constants

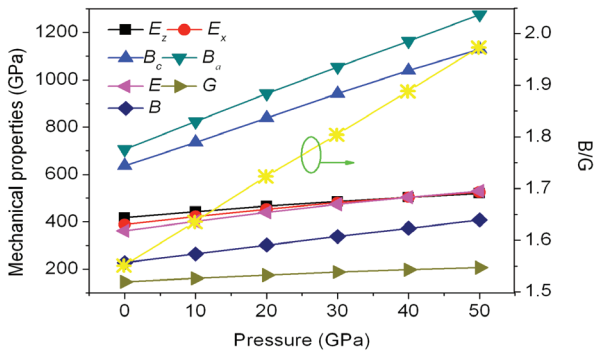

FIGURE 3. The pressure dependence of bulk modulus, shear modulus, Young's modulus, E_x, E_z, B_a, B_c and B/G

B_a/B_c with pressure indicates the weakening chemical bonding and the increasing anisotropy in this compound. The increases of B, G and E have comparatively slow with pressure.

ELECTRONIC PROPERTIES

Our calculated direct gap at Γ point of α-Al_2O_3 at 0 GPa and 0 K is 5.980 eV, which is consistent with the previous values of 5.82 eV (Matsunaga et al. 2003), 6.4 eV (Hosseini et al. 2005a) and 6.8 eV (Ru & Qiu 2009). However, these data are all smaller than the experiment of 8.7 eV (French 1990) due to the DFT underestimation. We cancel this underestimation here (this underestimation can be solved by scissors operator (Asahi et al. 2000)), but focus on the effects of pressure on the high symmetry points. Figure 4 shows the pressure dependence of the indirect and direct band gaps on the high symmetry points. These band gaps are calculated as a function of pressure to investigate the effects of pressure on the size of the energy gaps, which are shown in Figure 4. We can see that the eigenvalues all increase with the increase of pressure and the change of Γ–Γ is most obvious. The partial density of states of α-Al_2O_3 at 0 GPa and 0 K are shown in Figure 5, which show that the upper valence bands are composed of O-2p states hybridized

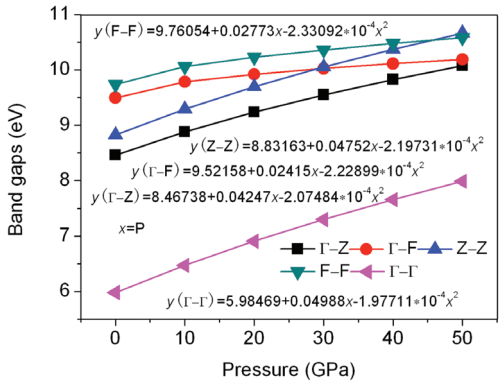

FIGURE 4. The pressure dependence of the indirect and direct band gaps on the high symmetry points

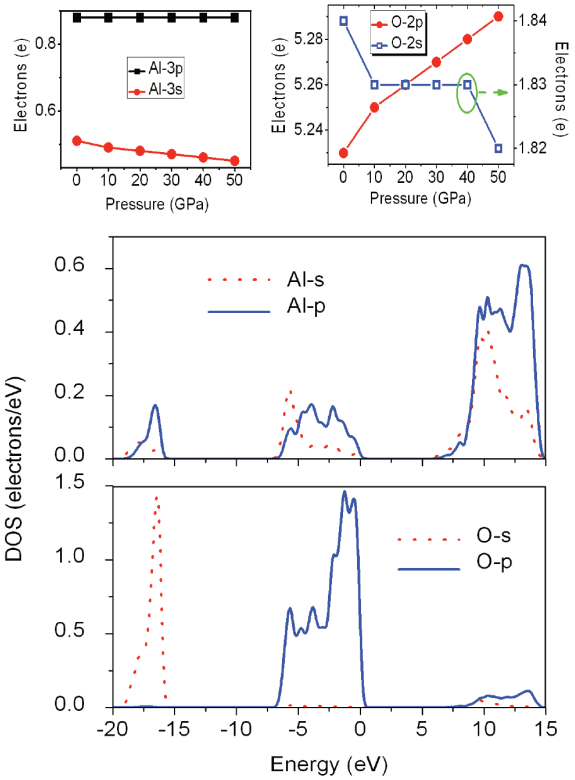

FIGURE 5. The partial density of states of α-Al_2O_3 at 0 GPa and 0 K along with atomic populations as pressure increases

with Al-3p and -3s states. The strong hybridization between Al and O induces comparatively high modulus. The atomic populations are shown in Figure 5 as pressure increases. We find the charge transfer from Al to O is about 1.61e, 1.62e, 1.64e, 1.65e, 1.66e and 1.67e from 0 to 50 GPa, which indicates the covalent bond weakens whereas the ionic bond strengthens. In Figure 5, the charge transfer is mainly between Al-3s and O-2p as pressure increases.

CONCLUSION

In summary, we have performed first-principles computations on α-Al_2O_3 including structural parameters, elastic, mechanical and electronic properties under pressure. The structural parameters obtained after relaxation are in agreement with previous experimental and theoretical data. The elastic constants, bulk modulus, shear modulus, Young' modulus, E_x, E_z, B_a, B_c and B/G all increase with increasing pressure. The result of B/G shows that there is a brittle-ductile transition at about 23.2 GPa. The anisotropy increases with increasing pressure. Moreover, band gaps and population analysis have been calculated as pressure increases.

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