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First-principles investigations of crystal structures and physical properties of jadeite under various pressures

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ABSTRACT

The crystal structures, electronic, elastic properties, hardness and phase transition of jadeite under various pressures from 0 to 70 GPa are investigated by using the first-principles calculations based on plane-wave pseudopotential density functional theory within the generalized gradient approximation (GGA). The calculated lattice parameters *a, b* and *c* were found perfectly agree with the available experimental data below 10 GPa. They all present linear responses to pressure until 60 GPa, lattice parameters present nonlinear variations. The calculation results show compression along *a*-axis is more difficult than that along *b*-axis or *c*-axis which can be explained by the alternative arrangement of Si—O tetrahedron and Al—O octahedron along *a*-axis. The elastic constants, bulk modulus, shear modulus, Young's modulus, *B/G*, Poisson's ratio, hardness and electronic properties are further investigated as a function of pressure which all present anomaly at 60 GPa. The generalized Born's mechanical stability criterion present jadeite is mechanical unstable above 62 GPa. The calculation results all present phase transition of jadeite occurs above 60 GPa, which agree with the available experimental data and other theoretical results.

1. Introduce

The alkali metal elements (K, Na) of oceanic crust and continental crust will subducted into the upper mantle and the transition zone. One of an important form of Na element accumulation in the mantle is Jadeite ($NaAlSi_2O_6$). In fact, the researches of monoclinic pyroxene compounds, for example, the stability and elastic properties of jadeite in ultra-high pressure can be a significant meaning of understand the fate of subducted crusts and the material formation in deep mantle.

Liu [1] first found jadeite will dissociate into an assemblage of the Calcium-Ferret type (CF) phase and stishovite in 1000 °C and 24 GPa by testing the quenched and decomposing products. Then CF was found in the basalt of mid-ocean ridge. The theoretical investigation of jadeite has not been deeply studied except Kawai and Tsuchiya [2] who studied $NaAlSi_2O_6$ jadeite, $NaAlSiO_4$ calcium ferrite (CF)-type phase and SiO_2 stishovite under the pressure of 0–30 GPa by the first-principles calculations, the result is in accordance with the experiment data [1].

Shock wave experiments on natural jadeite studied by McQueen et al. [3] up to 120 GPa, indicate probably no phase change up to about 70 GPa. Kesson et al. [4] reported the existence of a calcium ferrite phase containing a significant amount of $NaAlSiO_4$ in Mid Ocean Ridge Basalt (MORB) compositional system at pressures of 45–70 GPa. Takazawa et al. [5] investigate the phase transition by shock wave experiment find that jadeite transforms to garnet and ilmenite type structures at pressures over 60 GPa. The jadeite phase transition studies over 30 GPa in literature mainly focus on shock wave experiment which can provide phase transition data but the researches on electronic properties, elastic properties and optical properties are still missing. We hope to verify phase transition via first-principles calculations and study the electronic properties, elastic properties and optical properties in order to compensate for the lacking of theoretical research.

2. Calculation methods

All the work in this article is using CASTEP code [6] based on the density functional theory (DFT). The electronic exchange interactions are using the generalized gradient approximation of Perdew-Burke-Ernzerh for solid (GGA-PBEsol) [7]. The cut off energy of plan-wave is 750 eV ensures convergence in energy to within 2 meV. The *k*-points $7 \times 8 \times 8$ is also be estimated by the same way. Both cut-off energy and Monkhorst-Pack points are well convergence of the calculated structures and energies. The convergence criteria of structural optimization

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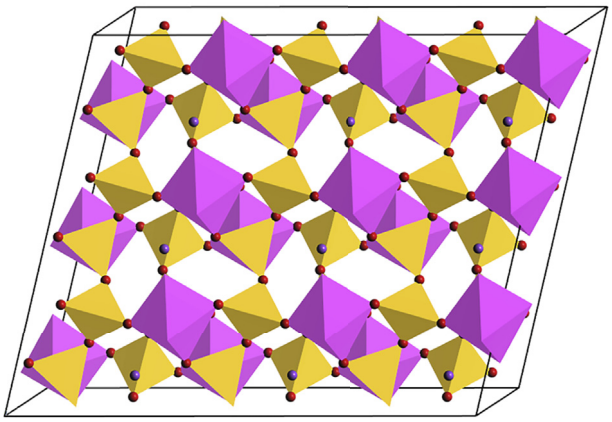

Fig. 1. The crystal structure of $NaAlSi_2O_6$ jadeite. The red spheres and purple spheres represent O and Na atoms, respectively. The yellow tetrahedron and pink octahedron represent the Si—O tetrahedron and Al—O octahedron respectively. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

were as follows: The energy change, maximum force, maximum stress and maximum displacement between optimization cycles which are 5×10^{-6} eV/atom, 0.01 eV/Å, 0.02 GPa, 5×10^{-4} Å respectively.

3. Results and discussions

3.1. Structure properties

The space group *C2/c* is considered to be the only structure of jadeite at high pressure. As show in Fig. 1, octahedrally coordinated aluminum polyhedral and tetrahedron coordinated silicate polyhedral run parallelly towards *c* axis, organizing a highly stable structure. The structure is so strong that the phase transition is difficult to happen in upper mantle. It is even harder to simulate the phase transition pressure by experiment. Hence all the jadeite experimental pressures are below 30 GPa. In contrast, the first-principle calculations can provide the methods to simulate the phase transition condition while other laboratory experiment is restricted in ultra-high pressure.

The calculated lattice parameters of jadeite are summarized in Table 1. The predicted lattice parameters up to 70 GPa of jadeite as well as experimental data from Nestola [8] are shown in Fig. 2a. From Fig. 2a we can obtain the calculated lattice parameters *a, b* and *c* fit the experimental data quite good. In other words, the first-principles calculations are convincing in predicting the lattice parameters under high pressure. From Table 1, we can see that the calculated values of lattice constants decrease slowly from 0 GPa to 60 GPa, then the lattice parameters curves show big dumps above 60 GPa. The lattice parameters anomaly indicates that the phase transition occurs at 60 GPa. Meanwhile, the lattice parameters *b, c* and angle β reduced rapidly but the increase of *a* at 60 GPa–70 GPa can provide the basis clue for the possible jadeite structure under high pressure.

Table 1
Lattice parameters under pressure from 0 GPa to 70 GPa.

Pressure (GPa)	Lattice parameters				
	a (Å)	*b* (Å)	*c* (Å)	β (°)	Volume (Å^3)
0	9.481	8.603	5.250	107.680	407.960
5	9.351	8.494	5.180	107.204	393.022
10	9.243	8.395	5.114	106.692	380.087
15	9.157	8.302	5.055	106.241	368.900
20	9.083	8.215	5.003	105.846	359.064
25	9.019	8.132	4.957	105.512	350.310
30	8.962	8.056	4.917	105.235	342.498
35	8.911	7.980	4.880	104.953	335.298
40	8.866	7.907	4.847	104.702	328.706
45	8.825	7.836	4.817	104.433	322.579
50	8.787	7.766	4.786	104.118	316.742
55	8.752	7.697	4.759	103.803	311.352
60	8.723	7.618	4.728	103.304	305.781
65	8.895	7.317	4.535	98.140	292.184
70	8.854	7.279	4.522	98.160	288.486

The pressure dependence of the normalized lattice parameters a/a_0, b/b_0, c/c_0, (a_0, b_0, and c_0 are the equilibrium lattice constants at 0 GPa) have been plotted in Fig. 2b. At low pressure range (P < 10 GPa), along the *a*-, *b*- and *c*-axis, the degrees of anti-compression along these three directions are almost the same. At high pressure range (P > 10 GPa), the decreasing rate of a/a_0 is smaller than that of b/b_0 and c/c_0 with increasing pressure, which means incompressibility along *a*-axis is larger than that along *b*- and *c*-axis. The structure of jadeite is that Si—O tetrahedron chains as well as Al—O octahedral chains all arrange along *c*-axis. And Si—O tetrahedron and Al—O octahedral arrange alternately in *a*-axis directions, forming a quasi-lamellar structure parallel to plane {100}. A pressure induced deformation along *a*-axis will be offset due to the different elastic properties between Si—O tetrahedron and Al—O octahedral under ultra-high pressure (P < 15 GPa), since the two different structures have different bulk modulus. In this way, the structure strength along *a*-axis will be enhanced, resulting the incompressibility along *a*-axis is larger than that along *b*- and *c*-axis at high pressure.

Both conventional lattice parameters and normalized lattice parameters show a data mutation at 60 GPa. It is easy to conclude that jadeite has a phase transition at 60 GPa, the crystal structure is definitely no longer C_2/c. The results are in good agreement with the shock wave experiments by Takazawa et al. [2], jadeite transformed into garnet and ilmenite type structures at pressures over 60 GPa.

3.2. Elastic properties

The calculated elastic constants of jadeite under pressure are present in Fig. 3. The calculations of jadeite elastic constants use the strain-stress method. We can obtain from Fig. 3 that crystal holds a quasi-linear dependence between the elastic constants and pressure in the range of 0–70 GPa. The longitudinal elastic constants C_{11}, C_{22}, C_{33} as well as shear elastic constants C_{44}, C_{55}, C_{66} are in good fit to each other consisting a positive value as a function of pressure. While the elastic constants C_{15}, C_{25}, C_{35} consist of a negative value, showing jadeite is a highly anisotropic material. It's also obvious all elastic constants have a non-linear change between 60 GPa and 65 GPa, especially depicted in longitudinal elastic constants and shear elastic constants which corresponds to lattice parameters change in 60–65 GPa.

3.3. Structure stability

The generalized Born's mechanical stability criterion of monoclinic phase at 0 GPa are given by Refs. [9,10]:

$$C_{ii} > 0,\ i = 1...6 \tag{1}$$

$$[C_{11} + C_{22} + C_{33} + 2(C_{12} + C_{13} + C_{23})] > 0 \tag{2}$$

$$(C_{33}C_{55} - C_{35}^2) > 0 \tag{3}$$

$$(C_{44}C_{66} - C_{46}^2) > 0 \tag{4}$$

$$(C_{22} + C_{33} - 2C_{23}) > 0 \tag{5}$$

$$[C_{22}(C_{33}C_{55} - C_{35}^2) + 2C_{23}C_{25}C_{35} - C_{23}^2C_{55} - C_{25}^2C_{33}] > 0 \tag{6}$$

$$\begin{aligned} 2[&C_{15}C_{25}(C_{33}C_{12} - C_{13}C_{23}) + C_{15}C_{35}(C_{22}C_{13} - C_{12}C_{23}) \\ &+ C_{25}C_{35}(C_{11}C_{23} - C_{12}C_{13})] - [C_{15}^2(C_{22}C_{33} - C_{23}^2) \\ &+ C_{25}^2(C_{11}C_{33} - C_{13}^2) + C_{35}^2(C_{11}C_{22} - C_{12}^2)] + C_{55}g > 0 \end{aligned} \tag{7}$$