Theoretical Calculation and Measurement of the Hardness of Diopside

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In the present paper, we test the suitability of a previously proposed model by Gao et al. for describing the hardness of more complicated, multicomponent crystals by both calculating and measuring the hardness of a diopside crystal. We analyze the limitations of the model and suggest that factors like load and temperature should be considered in the model. The calculated value of hardness of the diopside crystal is compared with the Vickers hardness values measured at different loads. A good agreement is found between the calculated hardness and the value measured at 25°C at a load of 0.5 N. Crystal orientation and measurement temperature have an impact on the experimental value of hardness of the crystals.

I. Introduction

Hardness is an important mechanical property for the application of various materials. A general definition of hardness is the mechanical resistance of a solid object to permanent change. Various experimental methods for determining hardness are available, e.g., Vickers, Brinell, Rockwell, and Knoop. The principle of these methods is to measure indentation hardness, i.e., a harder material is indented to a sample at a selected load with the size of the indented hole being related to the hardness of the crystal.

From an industrial point of view, it is desirable to predict the hardness of a new material before manufacturing. If prediction is feasible, it could furthermore contribute to the development of new superhard materials. A superhard material can be defined as a material with microhardness exceeding 40 GPa. The search for new superhard materials has attracted interest as superhard materials could be used as wear-resistant coating or as abrasive particles.

As no relationship between hardness and other macroscopic properties has been established, it is necessary to develop a method to directly calculate the hardness of a material. Some promising efforts have been made in the search for such a method. It has been established that bulk modulus can be related to the amount of bonds per volume. More importantly, a method for calculating hardness is developed by considering the strength of each individual bond and the amount of bonds per volume, i.e., on the first principle calculations of chemistry, Gao et al. have succeeded in calculating the hardness of covalent crystals, and concluded that hardness is an intrinsic property. The method is applicable for polar covalent crystals, oxide crystals with some ionic character, and nitride spinel. A crucial step of the method is to split the complex crystal into pseudobinary crystals, each containing only one chemical bond, using the approach proposed by Zhang.

Diopside (CuMgSi2O6) is in this work chosen as the example to study the validity of the approach of Gao et al. on complex minerals (containing more than three elements). If the method proposed by Gao et al. is proven to apply to diopside, by comparing the calculated data with the measured data, it would become possible for the method to be used for the hardness calculation of other complex minerals, i.e., the universality of the method would be strengthened. Moreover, diopside is chosen for the following two reasons. First, diopside is the dominant crystalline phase occurring in the heat-treated basaltic glasses and in many other heat-treated aluminosilicate systems. The diopside phase has a strong impact on the thermal and mechanical properties of those systems. Second, the crystallographic and bonding data are available in the literature. Another aim of this work is to discuss the limitations of the method and give suggestions for improvement.

II. Theory

In a multicomponent crystal (a crystal constituted by more than two different atoms), bonds are found between different atoms and the crystal thus consists of various chemical bonds. In Gao et al., the hardness of each individual chemical bond is calculated. Hence, before the calculation, the multicomponent crystal must be split into pseudobinary crystals containing only one chemical bond. The work described in Gao is based on the theoretical approach devolved by Zhang, which is expounded in the following section. Afterwards, the approach of Gao et al. and Gao is presented before the calculation of the hardness of diopside is carried out.

1) Decomposition into Pseudobinary Crystals

To perform the decomposition of a complex crystal, it is necessary to have information on the crystal structure plus crystallographic data revealing the different chemical bonds. As solely one chemical bond confines the pseudobinary crystal, the latter can be denoted as AaBb. Starting by considering atom A, it must be known which atom(s) A is bonded to in the multicomponent crystal. In addition, the following information must be available: (i) the number of B atoms that atom A is bonded to (N(B–A)); (ii) the nearest coordination number of A, i.e., the number of B atoms and other atoms that atom A is bonded to (N(CA)); and (iii) the number of A atoms in the pseudobinary crystal AaBb (a). The equivalent procedure must be applied when considering atom B.

When decomposing the multicomponent crystal, a number of pseudobinary crystals arise. The pseudobinary crystals can be added to give the composition of the entire multicomponent crystal. The pseudobinary crystals in the sum must be weighted according to how many times they are present in the multicomponent crystal. The weight of atom A in AaBb can be calculated.
by the following formula\textsuperscript{12}:
\[
\text{Weight of atom } A = \frac{N(B - A) \cdot a}{N_{CA}} (1)
\]

The weight of atom B in A\textsubscript{A}B\textsubscript{B} is calculated equivalently.

(2) Hardness of Each Pseudobinary Crystal

When indenting a material, rearrangement of atoms will occur in the indented area, i.e., electron–pair bonds must be broken and then reformed. When the bonds are broken, two unpaired electrons arising from the former bond exist. From an energetical point of view, this is equal to two electrons being excited from the valence band to the conduction band. Therefore, the activation energy required for plastic deformation is twice the band gap, \(E_G\).\textsuperscript{18} This mechanism of hardness is valid for covalent and polar covalent substances where bonding is localized.\textsuperscript{9} In this case, hardness is considered to be intrinsic by Gao \textit{et al.}\textsuperscript{9} and can be evaluated as the sum of the resistance of each bond per unit area.\textsuperscript{19} The resistance force of each bond can be described by the band gap and the valence electrons.

The hardness of a binary crystal composed of a \(\mu\) bond is calculated as follows:\textsuperscript{9}
\[
H_{\mu}^h (\text{GPa}) = A(N_{CA}^\mu) 2/3 E_{\mu}^h (2)
\]
where \(A\) is a constant and \(N_{CA}^\mu\) is the number of valence electrons per cubic Angstrom. Thus, hardness is calculated by the bond density and the strength of the bond. \(E_{\mu}^h\) can be substituted by \(E_{\mu}^p\) (the pure covalent contribution to \(E_{\mu}^h\) and \(f_{\mu}^i\) (ionicity))\textsuperscript{9}:
\[
H_{\mu}^h (\text{GPa}) = 0.630 A(N_{CA}^\mu) 2/3 e^{-3/\sigma} E_{\mu}^h (3)
\]
where \(\sigma\) is a constant. \(A\) and \(\sigma\) are determined by an experimental correlation between hardness and ionicity. Gao \textit{et al.}\textsuperscript{9} have found that \(A = 14\) and \(\sigma = 1.191\) when 10 crystals are used in the analysis. Therefore, Eq. (3) reduces to
\[
H_{\mu}^h (\text{GPa}) = 8.82(A N_{CA}^\mu) 2/3 e^{-1.191/\sigma} E_{\mu}^h (4)
\]

It should be noted that the hardness will only have the unit of GPa if \(N_{CA}^\mu\), \(E_{\mu}^h\), and \(f_{\mu}^i\) are inserted as \(\text{Å}^{-3}\), eV, and dimensionless, respectively. The various terms required for calculating the hardness of a pseudobinary crystal are described in Sections II(2)(A)–(C).

(A) Calculation of \(N_{CA}^\mu\): The calculation of \(N_{CA}^\mu\) requires knowledge of several parameters that will be calculated preliminarily. First, the number of effective valence electrons ((\(Z_{\mu}^n\))^\* must be calculated. When considering atoms without d-electrons, (\(Z_{\mu}^n\))^\* can be replaced by the number of valence electrons (\(Z_{\mu}^n\))^\*. With the knowledge of \((Z_{\mu}^n)^\*\) and \(N_{CA}\) (nearest coordination number) for both atom A and atom B, the number of effective valence electrons per \(\mu\) bond ((\(n_{CA}^\mu\))^\*) can be determined by Eq. (5).\textsuperscript{10}
\[
(n_{CA}^\mu)^* = (Z_{\mu}^a)^* / N_{CA} + (Z_{\mu}^b)^* / N_{CB} (5)
\]
Furthermore, the number of bonds per unit volume (\(N_{8\mu}\)) for each bond type must be known. This value can, e.g., be obtained by knowing the unit cell volume of the given crystal and the number of each bond type in the unit cell. \(N_{8\mu}\) is needed in the calculation of the bond volume (\(v_{\mu}^8\)):
\[
v_{\mu}^8 = \frac{(dv)^3}{\sum (dv)^3 N_{8\mu}} (6)
\]

where \(d\) is the bond length and \(v\) denotes an arbitrary bond in the multicomponent crystal. Now it is possible to calculate \(N_{8\mu}^\mu\):
\[
N_{8\mu}^\mu = (n_{CA}^\mu)^* / v_{\mu}^8 (7)
\]

(B) Calculation of \(E_{\mu}^h\): The calculation of \(E_{\mu}^h\) requires only the value of \(d_{21}\):
\[
E_{\mu}^h = \frac{39.74}{(dv)^{21}} (8)
\]
where the unit of \(E_{\mu}^h\) is eV if the unit of \(d_{21}\) is Å.

(C) Calculation of \(f_{\mu}^i\): Now, the decomposition of the multicomponent crystal is to be utilized. \(n\) is the ratio of atom B to atom A in the pseudobinary crystal. It is necessary to know \(n\) in order to calculate the average coordination number (\(N_{CA}^\mu\))\textsuperscript{10}:
\[
N_{CA}^\mu = N_{CA}/(1 + n) + n N_{CB}/(1 + n) (9)
\]

When \(N_{CA}^\mu\) is calculated, the structural correction factor \(b_{\mu}^1\) can be estimated:\textsuperscript{22}
\[
b_{\mu}^1 = \beta (N_{CA}^\mu)^2 (10)
\]
where \(\beta\) is a constant that can be estimated to 0.089 ±10%.\textsuperscript{22} Furthermore, the Thomas–Fermi screening wave number (\(k_{\mu}^1\)) of the valence electron in the \(\mu\) bond must be calculated:\textsuperscript{21}
\[
k_{\mu}^1 = \left( \frac{4 \sqrt{3} \pi^2 N_{CA}^\mu}{a_0 \rho \pi} \right)^{1/2} (11)
\]
where \(a_0\) is the constant Bohr radius (0.529 Å), \(b_{\mu}^1\) and \(k_{\mu}^1\) are utilized when calculating \(C_{\mu}\) (the ionic contribution to \(E_{\mu}^h\)):\textsuperscript{10}
\[
C_{\mu} = 14.4 b_{\mu}^1 |(Z_{\mu}^a)^* + \Delta Z_{\mu}^a| e^{-k_{\mu}^1 d_{21}} / r_{\mu}^1 (12)
\]
where \(\Delta Z_{\mu}^a\) is a correction factor that accounts for d-electron effects and \(r_{\mu}^1\) is half of the bond length. In Gao,\textsuperscript{10} the absolute value is not utilized, but this could lead to \(C_{\mu}\) having a nonsense negative value. \(Z_{\mu}^a\) denotes the number of valence electrons in the B anion and will be larger than \(Z_{\mu}^a\) as this denotes the number of valence electrons in the A cation. In the opinion of the authors, the value \(Z_{\mu}^a - n Z_{\mu}^a\) will never be positive. However, the sign of \(C_{\mu}\) is unimportant. The reason for this is that \(C_{\mu}\) is only used in the calculation of the ionicity, which can be expressed as follows:\textsuperscript{21}
\[
f_{\mu}^i = \frac{(C_{\mu})^2}{(E_{\mu}^h)^2 + (C_{\mu})^2} (13)
\]

(3) Hardness of a Multicomponent Crystal

The hardness (\(H_c\)) of a multicomponent crystal is a geometric average of all bonds in the pseudobinary crystals that accounts for the fact that soft bonds break before hard bonds. Therefore, it should be calculated as follows:\textsuperscript{5}
\[
H_c = \left( \prod_{\mu} (H_{\mu}^h)^{n_{\mu}} \right)^{1/\sum n_{\mu}} (14)
\]
where \(n_{\mu}\) is the number of \(\mu\) bonds comprising the multicomponent crystal.

(4) Calculating the Hardness of Diopside

Diopside is a monoclinic \(\text{C}_2\text{C}\) pyroxene with the cell dimensions 9.743, 8.923, and 5.251 Å for a, b, and c, respectively. \(\beta\) is 105.93°.23 The schematic microstructure is shown in Fig. 1.
From Cameron et al., 24 Rausdell et al., 25 Gordon et al., 26 and
Levin and Prewitt, 27 it is established that diopside has 11 different
types of bonds that all occur twice. Furthermore, the 6 ox-
ygens are different because they have different coordination
numbers and/or bind to different cations. Therefore, the oxygen
are all labeled, e.g., O(1). In contrast to this, Ca, Mg, and Si
have constant coordination numbers and only bind to oxygen.
Table I assembles the information about the different bonds in
diopside and the length of the bonds.

(A) Decomposition of Diopside into Pseudobinary Crystal
Subformulas: By applying Eq. (1) to all the bond types present-
ated in Table I, the following decomposition of diopside is obtained:

\[
\text{CaMgSiO}_6 = \text{CaMgSiO}_6(O(1)) + \text{CaMgSi}_2O(2)) + O(3)) + O(3')
\]

As diopside has been split into pseudobinary crystals, the
hardness of each bond can be calculated. The calculation of the
hardness of the CaO(1) bond will exemplify the methodology.
Afterwards, the bond parameters of the other bonds, which
are used for calculating the overall hardness, will be presented
in Table II.

(B) Bond Parameters for Diopside: Ca and O have no
d-electrons and therefore \(Z^d_{Ca} = 2\) and \(Z^d_{O} = 6\). As
Ca is bonded to 8 oxygen, \(N_{Ca} = 8\), and as \(O(1)\) is bonded to
one Ca, Mg, and Si, \(N_{O(1)} = 3\). According to Eq. (5), \(m^d_{Ca}\)
is then 2.25. As all the bonds in diopside occur with the same
frequency per unit volume, \(N_{b}\) is constant for all the bonds in
diopside. By counting the number of bonds in the unit cell of
diopside (cf. Table I), \(N_{b}\) can be calculated by dividing this
number (2) with the unit cell volume \(438.97 \cdot 4.77\). That is,
\(N_{b} = 4.556 \cdot 10^{-3} \text{ Å}^{-3}\). For \(CaO(1)\), \(N_{CaO(1)}\) can then be calculated
using the bond length given in Table I and by insertion into
Eq. (6). This gives \(N_{CaO(1)} = 26.93 \cdot 4.71 \text{ eV}\). Therefore, \(N_{CaO(1)}\) is:

\[
N_{CaO(1)} = 225/26.93 = 0.0836 \quad \text{Å}^{-3}
\]

With a bond length of 2.363 Å for \(CaO(1)\), \(E_{CaO(1)}\) is calculated
according to Eq. (8):

\[
E_{CaO(1)} = 39.74 \text{ eV} \cdot \text{Å}^{-2.48} = 4.71 \text{ eV}
\]

The next step is the calculation of \(f^d_{CaO(1)}\). According to Eq.
(15), the ratio between O(1) and Ca is \(4/3\) (i.e., \(n = 4/3\)). All
the information needed to calculate \(N_{CaO(1)}\) by Eq. (9) is now available:

\[
N_{CaO(1)} = 5.14. This value can directly be used to calculate
\(f^d_{CaO(1)}\) to be 2.35 using Eq. (10), \(f^d_{CaO(1)}\) is then calculated
to be 1.80 Å⁻¹ using Eq. (11). This and other now-known values are
inserted into Eq. (12) and \(C_{CaO(1)}\) is determined to 20.4 eV. By

Table I. Bond Types and Lengths in Diopside

<table>
<thead>
<tr>
<th>Center atom</th>
<th>Bond type (Å)</th>
<th>N</th>
<th>Bond length (Å)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ca</td>
<td>CaO(1)</td>
<td>2</td>
<td>2.363</td>
</tr>
<tr>
<td></td>
<td>CaO(2)</td>
<td>2</td>
<td>2.347</td>
</tr>
<tr>
<td></td>
<td>CaO(3)</td>
<td>2</td>
<td>2.561</td>
</tr>
<tr>
<td></td>
<td>CaO(3')</td>
<td>2</td>
<td>2.721</td>
</tr>
<tr>
<td>Mg</td>
<td>MgO(1)</td>
<td>2</td>
<td>2.119</td>
</tr>
<tr>
<td></td>
<td>MgO(1')</td>
<td>2</td>
<td>2.061</td>
</tr>
<tr>
<td></td>
<td>MgO(2')</td>
<td>2</td>
<td>2.051</td>
</tr>
<tr>
<td>Si</td>
<td>SiO(1)</td>
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<td>1.602</td>
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<tr>
<td></td>
<td>SiO(2)</td>
<td>1</td>
<td>1.589</td>
</tr>
<tr>
<td></td>
<td>SiO(3)</td>
<td>1</td>
<td>1.669</td>
</tr>
<tr>
<td></td>
<td>SiO(3')</td>
<td>1</td>
<td>1.687</td>
</tr>
<tr>
<td>O(1)</td>
<td>O(1)Ca</td>
<td>1</td>
<td>2.363</td>
</tr>
<tr>
<td></td>
<td>O(1)Mg</td>
<td>1</td>
<td>2.119</td>
</tr>
<tr>
<td></td>
<td>O(1)Si</td>
<td>1</td>
<td>1.602</td>
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<td>O(3)Si</td>
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</tr>
<tr>
<td></td>
<td>O(3)Si(1)</td>
<td>2</td>
<td>1.687</td>
</tr>
</tbody>
</table>

The bond lengths are given at room temperature. \(N_{b}\) is the number of a specific ligand that is bonded to the central atom.

Table II. Bond Parameters for the Bonds Confining Diopside

<table>
<thead>
<tr>
<th>Bond type (μ)</th>
<th>(N_{b}^d) (Å⁻¹)</th>
<th>(E_{b}^d) (eV)</th>
<th>(f_{b}^d) (-)</th>
<th>(H_{b}^d) (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CaO(1)</td>
<td>0.0836</td>
<td>4.71</td>
<td>0.949</td>
<td>2.56</td>
</tr>
<tr>
<td>CaO(2)</td>
<td>0.0663</td>
<td>4.79</td>
<td>0.977</td>
<td>2.16</td>
</tr>
<tr>
<td>CaO(3)</td>
<td>0.0510</td>
<td>3.86</td>
<td>0.978</td>
<td>1.46</td>
</tr>
<tr>
<td>CaO(3')</td>
<td>0.0426</td>
<td>3.32</td>
<td>0.979</td>
<td>1.11</td>
</tr>
<tr>
<td>MgO(1)</td>
<td>0.120</td>
<td>6.17</td>
<td>0.831</td>
<td>5.04</td>
</tr>
<tr>
<td>MgO(1')</td>
<td>0.354</td>
<td>6.61</td>
<td>0.672</td>
<td>13.1</td>
</tr>
<tr>
<td>MgO(2')</td>
<td>0.360</td>
<td>6.69</td>
<td>0.671</td>
<td>13.4</td>
</tr>
<tr>
<td>SiO(1)</td>
<td>0.358</td>
<td>12.3</td>
<td>0</td>
<td>54.9</td>
</tr>
<tr>
<td>SiO(2)</td>
<td>0.305</td>
<td>12.6</td>
<td>0.323</td>
<td>34.3</td>
</tr>
<tr>
<td>SiO(3)</td>
<td>0.263</td>
<td>11.2</td>
<td>0.326</td>
<td>27.1</td>
</tr>
<tr>
<td>SiO(3')</td>
<td>0.255</td>
<td>10.9</td>
<td>0.339</td>
<td>25.7</td>
</tr>
</tbody>
</table>
solving $C^{\text{CaO}(1)}$ and $E_h^{\text{CaO}(1)}, f_{i}^{\text{CaO}(1)}$ can be determined to be:

$$f_{i}^{\text{CaO}(1)} = \frac{(20.4 \text{ eV})^2}{(20.4 \text{ eV})^2 + (4.71 \text{ eV})^2} = 0.949$$

(18)

The hardness of the CaO(1) bond is calculated:

$$H_{c}^{\text{CaO}(1)} = 8.82 \frac{\text{GPa} \cdot \text{Å}^2}{\text{eV}} \cdot (0.0863 \text{ Å}^{-1})^{3/2} \cdot 4.71 \text{ eV} \cdot e^{-1.19 \times 0.949} = 2.56 \text{ GPa}$$

(19)

The bond parameters for all 11 bonds in diopside are listed in Table II. It can be observed that the SiO bonds are the hardest because of their covalent nature.

The hardness of the multicomponent crystal diopside can be calculated. This is done by inserting the hardness of the pseudo-binary crystals given in Table II into Eq. (14). All hardness values are given in GPa and $n^{th}$ as all bonds occur twice in CaMgSi$_2$O$_6$.

$$H = \frac{(2.56^2 \cdot 1.67^2 \cdot 1.46^2 \cdot 1.11^2 \cdot 5.04^2 \cdot 13.1^2 \cdot 13.4^2 \cdot 54.9^2 \cdot 34.3^2 \cdot 27.1^2 \cdot 25.7^2)^{1/22}}{2} = 8.15 \text{ GPa}$$

(20)

The calculated value is the geometric average. The weighted average hardness of the bonds in Table II is 16.4 GPa. This shows that the soft bonds are of greater importance to the overall hardness than the strong bonds.

### III. Experimental Procedure

Two samples from a diopside mineral (from the state of Minas Gerais in Brazil) were cut into samples with dimensions of 3.0 $\times$ 1.5 $\times$ 1.0 cm$^3$ using a Secotom-10 diamond-coated blade (Struers A/S, Ballerup, Denmark). One of the samples was heat treated in a furnace (K10, Scandinavien A/S, Alleroed, Denmark) at 1100°C for 30 min under atmospheric conditions and subsequently exposed to room temperature. Both samples were ground and polished with LaboPol-5 (Struers). The final step of the polishing was carried out using silicon carbide paper with a grit size of P4000 (Struers).

Vickers microhardness was measured using a Duramin indenter (Struers). All indentations had a duration of 5 seconds. The hardness of the heat-treated sample was measured 40 times at 0.49 N. The other sample was measured at 0.25, 0.49, 0.98, and 1.96 N, with 40 measurements at each load. The choice of the loads and the number of repetitions have been considered in accordance with the issues described by Quinn and Quinn.²⁸

### IV. Results and Discussion

Figure 2 shows the dependence of the hardness of the untreated diopside on load applied during indentation. The hardness of the heat-treated diopside was measured at 0.49 N. The development of hardness against load has been fitted using Kick’s law.²⁵ Kick’s law is not theoretically applicable to Vickers hardness as it was developed for the Brinell test, but can anyway provide a good empirical fit to Vickers hardness measurements.²⁷ Kick’s law is stated as follows:

$$P = C \cdot d^n$$

(21)

where $P$ is the load, $C$ is a constant, $d$ is the measured impression size, and $n$ is the logarithmic exponent. By definition, hardness is²⁸:

$$H = \frac{P}{d^2} = \frac{C d^n}{d^2}$$

(22)

where $z$ is dependent on the indenter geometry.
account in the method described in Section II(2). Using the work of Cameron et al., the bond lengths and unit cell volume against temperature have been linearly extrapolated to 1100°C. The hardness of diopside in an inert atmosphere at 1100°C can be calculated to be 7.71 GPa. Dorner and Stückert have measured the Vickers hardness of diopside to be 4.9–6.1 GPa at temperatures between 300°C and 750°C with a load of 0.5 N. Their values are 2–3 GPa lower than the hardness reported here. The discrepancy can, in addition to the elevated temperature, be ascribed to a loading period of 10 s, which is longer than that used in the present work.

In crystals, the different planes can contain different bonds and therefore the hardness of a crystal may be dependent on the orientation of the crystal concerning the Miller indices. This has, for instance, been experimentally confirmed for SiC and MgO. The crystal orientation effect is not accounted for in the calculation method. Starting from the measured hardness of diopside, this value does not seem to be influenced by the orientation as the standard deviation is rather low. This can arise from two factors. Firstly, the indentation can be an average hardness of many microcrystals. Secondly, the hardness of diopside is only weakly dependent on crystal orientation, which has been confirmed at elevated temperatures. In cases where the conditions are not fulfilled, the crystallographic data used in the hardness calculation must arise from the same orientation in which the indentation is performed.

It is important to recall that the calculated hardness is associated with uncertainty as the parameter β has an uncertainty of 10%. This results in a change in the calculated hardness of 3% for the case of diopside. Furthermore, the empirical fit leading to the parameters α and A of Eq. (4) is associated with uncertainty. In particular, the utilization of SiC as one of 10 crystals in the fit approximation to calculate the hardness of multicomponent crystals. In order for the model to be more precise, we suggest reestablishing the hardness calculation must arise from the same orientation in which the indentation is performed.

V. Conclusion

The hardness of diopside has been calculated to be 8.15 GPa, which is in accordance with the measured values. This indicates that the calculation method is applicable to complicated crystals such as pyroxenes even though they possess some ionic character. Therefore, the model proposed by Gao et al. can be a good approximation to calculate the hardness of multicomponent crystals. In order for the model to be more precise, we suggest that the load, geometry, and temperature dependency of hardness should be specified in the model. The temperature dependence of the unit cell volume is discussed. The calculated and measured indentation hardness must be compared for the same load and crystal orientation.

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References


