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Methodology Article

How to Estimate Bulk Modulus and Phonon Frequency of a Crystal from Numerical Values of Vickers Hardness Expressed in GPa

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Abstract

Several empirical formulas based on the bulk and shear moduli of crystals have been proposed to calculate hardness, but the mathematical expressions usually do not correspond to the units in GPa measured experimentally. The aim of this work is to reveal the relationship between measured and calculated units and to find quantities that could be derived from the numerical values of Vickers hardness measured experimentally in GPa. For this purpose, bond strength model of hardness is applied because it establishes a quantitative relationship between macroscopic hardness and the bonding characteristics in a crystal. It is shown that experimental GPa values of Vickers hardness is proportional to the magnitude of interatomic force densities calculated in [N/m^3]. Hardness corresponds to the average of all interatomic forces, but in crystals where all interatomic forces are equal, hardness is directly proportional to this force. This work shows how to derive the magnitude of interatomic forces from experimental Vickers hardness values in the crystals with tetrahedrally coordinated structures, NaCl-like, CsCl-like or NiAs-like structures, and how to apply these forces to estimate the bulk moduli and phonon frequencies of these materials. For zinc-blende type structures quantitative results are compared with experimental data for typical A^{III}-B^{V} crystals.

Keywords

Hardness, Bonding, Strength, Crystal, Calculations, Phonons

1. Introduction

Hardness can be defined as a material's resistance to permanent deformation; it is also referred to as resistance to scratching, wear, or cutting [1]. Indentation hardness is defined as a material's resistance to indentation. The resulting impression is measured using a method-specific procedure with a scale of values defined by the testing method, e.g., Rockwell, Brinell, Vickers, or Knoop hardness. These methods now provide quantitative data on the hardness of a material, and numerical results allow for a quantitative comparison of hardness of different materials. The Vickers number Hv is measured according to the size of the indentation and is calculated using the formula Hv = 1.854(F/A), where F is the applied load and A is the area of the indentation. Therefore, Hv is measured in units of pressure, i.e., in pascals, usually in GPa. The resulting numbers are quantitative technical values suitable for a comparing the hardness of different materials, however, they have not yet been used to study other properties of materials.

From graphs of hardness versus bulk modulus B or shear modulus G, a tendency of positive correlation was observed, indicating that a hard material should have a high bulk modulus to resist

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volume reduction under applied load, and a high shear modulus to limit deformation in directions other than that of the applied load. Therefore, several models have been proposed to calculate hardness based on the material's B and G values. For example, the most successful equations for estimating hardness are [2, 3]:

$$H_v = 2(k^2\ G)^{0.585} - 3,\ \text{Chen model} \quad (1)$$

$$H_v = 0.92\ k^{1.137}\ G^{0.708},\ \text{Tian model} \quad (2)$$

where k=G/B is the Pugh's modulus. The parameters in the models were obtained by an empirical fit to experimental measurements for many systems to obtain H_v results in GPa units, however, it is evident that the mathematical expressions (1), (2) do not correspond to the unit of GPa. Nevertheless, the models present their resulting numbers in GPa which is necessary for comparison with measured data in GPa. The aim of this work is to uncover a relationship between the measured GPa and calculated SI units and find quantities that could be derived from experimental Vickers hardness GPa numerical values.

The systematic search for new hard materials has led to various practical recipe constructions that yield reasonable results and predictive capabilities. Semi-empirical hardness models achieve values that correspond surprisingly well with experimental data [4-11]. The results of all calculations are presented in GPa units as formulas (1) and (2) for the purpose of comparison with experiments, despite the units resulting from the semi-empirical formulas. Among these models, the bond strength model [5] establishes a quantitative relationship between macroscopic hardness and microscopic quantities in samples. In addition, this model had previously demonstrated excellent performance in purely covalent solids as well as in transition metal carbide and nitride systems [12]. An important advantage of this model is its clear physical meaning and microscopic interpretability: it establishes a quantitative relationship between macroscopic hardness and the bonding characteristics in a crystal [13]. For these reasons, we apply the bond strength model [14]. here to determine the SI unit of the calculation.

2. Methodology

The original form of the method [5] assumes localized bonding electrons in a covalent or polar-covalent bond, the same inter-atomic distances d_{ij} between atom *i* and all its nearest neighboring atoms *j*, and defines the bond strength s(ij) between atom *i* and atom *j* as

$$s(ij) = \frac{1}{n_i\ n_j}\frac{\sqrt{e_ie_j}}{d_{ij}}\ e^{-\sigma f_{ij}} \quad (3)$$

where n_i and n_j are the coordination numbers of atoms *i*, *j*, $e_i = Z_i\ /R_i$ and $e_j = Z_j\ /R_j$, and d_{ij} are inter-atomic distances between atom *i* and its nearest neighboring atoms *j*. The charges Z_i, Z_j correspond to the number of valence electrons of atoms *i*, and *j*, and R_i, R_j are the radii of atoms *i*, and *j*. The reference energy e_i of the atom *i*, is the potential of the individual atom *i* to attract the valence charge of the crystal. When there are differences in the potentials e_i and e_j of atoms in a bond, the tendency for bond breaking increases in the presence of a "weaker partner" in the bond. The effect of the difference between e_i and e_j is phenomenologically described by an exponential factor $e^{-\sigma f_{ij}}$, where $f_{ij} = ((e_i - e_i)/(e_i + e_j))^2$. The resulting Vickers hardness H_V (bs) has the form

$$Hv(\mathrm{bs}) = C\frac{N}{\Omega}\ \left[\prod_{ij}^{N} s(ij)\right]^{\frac{1}{N}} \quad (4)$$

where N is the number of all bond strengths s(ij) in the volume Ω. The bond strength model formula for H_V (bs) is the volume density of interatomic bonds multiplied by the geometrical average of N bonds in the corresponding volume Ω.

In principle, all quantities in Eqs. (3), (4) are accessible through first-principles method [5], however, in this work we determine e_i, and e_j, using the Pearson's [15] valence and atomic radii of the elements, which are also published in Kittel's textbook [16]. Then the coefficient C=1450 is chosen so that it couples calculated values H_V with the experimental hardness values of silicon measured in GPa, assuming all distances (i.e., R_i and d_{ij}) are measured in angstroms. The coefficient σ = 2.8 was adjusted according to the measured hardness of SiC, AlN and GaAs crystallizing in zinc blend structure [14]. These values C=1450 and σ = 2.8 were used for different crystals in all applications of the bond strength method, in this work the value C=1450 is not used.

In diamond-like or in zinc blend crystal structure, there is only one distance $d = d_{ij}$, $n_i = n_j = n = 4$, N=16 and one type of bond strength s(ij), which simplifies formula (4) so that

$$Hv(bs) = \frac{C}{\Omega}N\ \ s(ij) = \frac{C}{\Omega}\ \frac{\sqrt{e_ie_j}}{d}\ \ e^{-\sigma f_{ij}} \quad (5)$$

To determine the physical unit of the bond strength method, all distances in eq. (5) should be in meters, the electron charge in coulombs, and the coefficient C=1 in Eq. (5). For the determination of units, the exponential factor is not necessary. Therefore, it is sufficient to evaluate

$$D(\mathrm{bs}) = \frac{1}{\Omega}\ \frac{\sqrt{e_ie_j}}{d} \quad (6)$$

The resulting D(bs) numbers in eq. (6) are enormous; the values are D(bs) = $761*10^{18}$ [N/m^3] for diamond and D(bs) = $98.3*10^{18}$ [N/m^3] for silicon. In atomic terms, it is more practical to use nanometers for distances and cubic nanometers (nm)^3 for volume Ω. Then, in nano-units D(bs) = 761 [nN/(nm)^3] and D(bs) = 98.3 [nN/(nm)^3] for diamond and silicon, respectively. The result is that the physical unit of D(bs) is the volume density of elastic force D(bs) [N/m^3] or D(bs) [nN/(nm)^3]. In the following text, nano-units are used.

Bulk modulus and hardness are related to interatomic forces. To find their mutual relations we initially use eqs. (5) and (6) so, that generally

$$Hv = C \;\; D \;\; e^{-\sigma f_{ij}}$$

where D is the volume density of interatomic forces and C is adjusted to Vickers hardness in GPa units.

Bulk modulus B is determined by interatomic forces and a reaction of the atomic positions to the external force. In diamond-like or in zinc blend crystal structure, atoms are bonded with n=4 bonds with neighbors, so B corresponds to four interatomic forces. Analogously with eq. (6) density of interatomic forces can be expressed as

$$D(B) = \frac{1}{n} \;\; \frac{B}{d} \qquad (7)$$

The resulting numbers for diamond are D(B) = 702 [nN/(nm)^3] and for silicon D(B) = 94.7 [nN/(nm)^3]. Since the interatomic forces in the D(bs) are determined by valence and the atomic radii of the constituting atoms, whereas D(B) is determined by the interatomic forces in the bulk modulus of solid, the densities D(bs) are in a remarkable accordance with D(B).

For comparison with experimental hardness values, the exponential factor $e^{-\sigma f_{ij}}$ omitted in eqs. (6) and (7) is restored (see eqs. (5), (6)), and C is adjusted to Vickers hardness of silicon H_V(exp) =12.0 GPa.

Then Vickers hardness H_V can be expressed in the forms

$$H_V(bs) = C(bs)\, D(bs)\; e^{-\sigma f_{ij}}\;,\; H_V(B) = C(B)\;\; D(B)\; e^{-\sigma f_{ij}}\;,\; \text{and } H_V(exp) = C(H)\;\; D(H)\; e^{-\sigma f_{ij}} \qquad (8)$$

where C (bs) = 0.1221 and C(B) = 0.1267.

These equations show that the Vickers hardness H_v (bs) and H_v (B) are calculated in units of [N/m^3] or [nN/(nm)^3].

Eq. (8) can be rewritten in the form

$$D(H) = H_V(exp)\; e^{\sigma f_{ij}} \;/C(H) \qquad (9)$$

where C(H)=0.124 is an average value of C_v (bs)=0.1221 and C_v(B)=0.1267. This equation directly determinates *D(H)* density of forces by means experimental Vickers hardness. Since the densities D(H), D(B) or D(bs) should not depend on the methods of calculations or measurements, from eq, (7) follows

$$B = D(B)\; n\; d = D(H)\; n\; d = H_V(exp)\; e^{\sigma f_{ij}} \quad n \;\; d \;\; /C(H)$$

$$\text{or } B(H) = H_V(exp)\; e^{\sigma f_{ij}} \quad n \;\; d \;\; /C(H).$$

Therefore, bulk modulus B can be expressed by experimental value H_v (exp) of Vickers hardness. The question arises whether the calculated interatomic force densities D(bs), D(B) and D(H) have any real physical significance.

Let us consider the elastic vibration of a diatomic linear chain with two atoms in with two masses M1 and M2. We define the forces F_a(bs) and F_a(B) such that

$$F_a(bs) = \frac{D(bs)}{k} \;\; F_a\,(B) = \frac{D(B)}{k} \;\text{ or }\; F_a\,(H) = \frac{D(H)}{k} \qquad (10)$$

where F_a is an interatomic elastic force acting on a single atom, and k is the number of atoms in the volume of one (nm)^3. Again, in principle, this should be $F_a(bs) = F_a\ (B) = F_a\ (H) = F$. The typical frequency of an elastic wave in terms of elastic constants is given for the optical branch [16] as

$$\omega^2 = 2F\left(\frac{1}{M1} + \frac{1}{M2}\right) = \frac{2F}{M},\; M = \frac{M1 * M2}{M1 + M2} \qquad (11)$$

For example, in the AlN crystal, there are 96.5 atoms per cubic (nm)^3, i.e., k=96.5, the reduced mass M=1.53*10^{-26} kg, and the force constant F_a(H) = 2.77 [nN], therefore, ω^2 = 2*2.77/1.53/10^{-26} = 3.621/10^{-26}. Then ω = 1.90*10^{13}, i.e., ω =19.0 THz.

In the case of SiC, ω^2 = 2*3.134/1.394/10^{-26} = 4.496*10^{26,} i.e., ω = 21.2 THz.

3. Results

The SI unit in eqs. (5)-(7) is the volume density of force [N/m^3] or [nN/(nm)^3]. The forces in eq. (6) correspond to elastic interatomic forces calculated from atomic parameters of constituent atoms and the crystal structure. They are quantitatively in good accordance with the elastic forces derived from the bulk moduli of the crystals in eq. (7). To verify the physical significance of the density of forces, these forces were applied in a model calculation of the crystal vibrations.

Vickers hardness is a measure of plastic deformation produced by indentation; however, the calculated densities D(bs) and D(B) correspond to elastic interatomic forces. For comparison with experimental hardness values, the exponential factor $e^{-\sigma f_{ij}}$ and the proportionality coefficients C(H) introduced in eqs. (8), (9) link the calculations with the experiment. The results of all calculations are presented in Table 1.

It is known that experimental hardness values depend on the measurement techniques as well as load, load-independent region, sample microstructure, temperature, etc. which may explain the variation in the corresponding data. For the use of the consistent experimental data in this work, data from the ref. [16] are used for hardness and bulk modulus B. Here, the results of the hardness models Cheng [2] and Tian [3] equations (1) and (2) are also presented and can be used for comparison with the results of H_v (bs) and H_v (B). The phonon frequencies are from ref. [18].

Experimentally, Vickers hardness is calculated from the size of the indentation, that is, from the area of the dent, using the formula Hv ~ F/A, where F is the applied force and A is the area of the indentation. In fact, the applied force F destroys the sample in certain volume and, therefore, the unit volume density of force is not surprising.

Table 1. *B, B(H)-bulk moduli [GPa], D(B), D(bs), D(H) - density of force [nN/(nm)^3], H_v(B), H_v(bs), H_v(exp) - hardness [GPa], F_a(H) -force [nN], and frequency ω(H) [s^{-1}] calculated from experimental value H_v (exp), ω(exp) is typical experimental value. Experimental data used for hardness and bulk modulus B are from the ref. [17], the phonon frequencies ω(exp) are from ref. [18].*

Crystal	B(exp)	B(H)	D(B)	D(bs)	D(H)	H_v(B)	H_v(bs)	H_v(exp)	Fa(H)	ω(H)	ω(exp)
Diamond	434	478	703	761	786	89.0	92.9	96.0	4.39	30.0	35 – 40
BN	372	428	595	689	695	58.6	65.4	66.0	4.11	28.5	31 – 36
SiC	212	226	282	287	305	32.6	32.0	34.0	3.13	21.2	24 – 29
AlN	195	200	257	267	267	17.9	18.0	18.0	2.77	19.0	18 – 20
GaN	175	169	225	240	221	16.0	16.4	15.1	2.51	16.1	17 – 22
Si	89	91	95	98	98	12.0	12.0	12.0	1.97	13.0	15 – 15.7
AlP	83	93	88	91	100	8.6	8.6	9.5	2.03	13.0	12 – 13.3
GaAs	63	71	64	76	74	6.7	7.7	7.5	1.67	7.2	8.2 – 8.3

4. Summary

The relationship between the measured Vicker hardness in GPa and calculated nN/(nm)^3 units is presented. It is shown how to derive the magnitude of interatomic force densities D(H) from experimental Vickers hardness values and how to apply D(H) to estimate the phonon frequencies of typical A^{III}-B^{V} crystals. The densities D(B) derived from the bulk modulus values of materials, the densities D(bs) derived from atomic parameters of constituent atoms, and the densities D(H) derived from experimental Vickers hardness data calculated in units of [N/m^3] or [nN/(nm)^3] are in good mutual accordance. The results demonstrate that hardness can be described by elastic interatomic forces modified by a factor approximating plastic deformation during hardness measurement. To verify the physical meaning of the volume density of forces, these forces were applied in a model calculation of crystal vibrations. Considering the simplicity of this approach and all approximations used, the quantitative accordance between all densities D(bs), D(B), D(H) and typical experimental frequencies with the calculations is acceptable.

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Data Availability Statement

I obtained the experimental data on hardness H(exp) and bulk modules B from references [14] and [15].

Conflicts of Interest

There are no conflicts to declare.

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