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Ultimate strength and brittleness of crystal solids

ALEXANDER S. BALANKIN
Instituto Tecnológico y de Estudios Superiores de Monterrey
Campus Estado de México, México

AND

ALEXANDER D. IZOTOV
Kurnakov Institute of General and Inorganic Chemistry, Moscow

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ABSTRACT. A Frenkel-Kontorova dislocation model variation is employed to construct a Hamiltonian, which in turn is used to compute the temperature dependence of ultimate tensile and shear stresses of crystal solids. A new brittleness parameter is also suggested. It is shown that with the proposed model one is able to predict the nature of a crystal (brittle, quasi-brittle, ductile, quasi-ductile) and estimate its ultimate strength.

RESUMEN. Mediante el empleo de una variación del modelo de dislocaciones de Frenkel-Kontorova se construye un nuevo hamiltoniano, que permite calcular la dependencia con respecto a la temperatura de la resistencia máxima a la tensión y el esfuerzo de corte para cristales sólidos. Con este nuevo modelo se sugiere una expresión para el parámetro de fragilidad. También se muestra que con el modelo propuesto es posible predecir la naturaleza de algunos cristales (frágil, cuasi-frágil, dúctil, cuasi-dúctil) y estimar su máxima resistencia.

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The behavior of materials offers an almost infinite variety of challenges in the quest of understand physical effects. Under ideal circumstances one would wish to start with an atomic or molecular model of the material and then construct a completely general theory of behavior that transcends all length scales of possible phenomena. With a profound understanding of this type, full scale macroscopic behavior of materials could be predicted from minimal and fundamental parameters of the material.

The first investigations devoted to the theoretical strength of crystals within the framework of quantum physics considered ideal cleavage in the sense that neighboring planes of the atomic lattice were assumed to be separated (see, for example, references in [2, 3]). This led to an estimation of the ultimate tensile stress, σ_C, which in fact exceeded by far those measured under ordinary conditions. Moreover, pure metals, like cooper or aluminum, are truly ductile materials which apparently cannot sustain a cleavage crack, but may fail by plastic instability and necking on a gross scale.

In his notable work [4], Frenkel first made a famous investigation into theoretical strength of ductile metals and also found a value of the shear strength, τ_C, higher by many orders of magnitude than the observed flow stresses of metals.[1] The original Frenkel model [4] is associated with the sliding of one semi-infinite half crystal over another and thus gives no way to estimate the tensile strength associated with cleavage fracture.

According to modern quantum-mechanical models of solid fracture (see Refs. [1, 5, 6] and references therein) crystal solids will be either brittle or ductile depending upon the ratio τ_C/σ_C. In fact, however, the ductile response of the solid is associated with the processes of dislocation production and propagation [6–9]. Because of this, shear strength of a deformed crystal is strongly dependent on the actual dislocation processes. On the other hand, even a low defect concentration catastrophically affects the tensile strength of a brittle crystal [2, 3]. Thus theoretical threshold stresses are rarely realized in practice.

Nonetheless, the theoretical ultimate strength of a crystal is of interest in solid physics and mechanics. First, theoretical ultimate strength is an important concept in the physical theory of deformed solids and is a material parameter central to modern theories of plasticity and fracture [6, 10–13]. Secondly, ultimate strength is the upper limit of the strength which can be reached in crystal solids under certain conditions.[2]

Various theoretical models of ultimate strength for crystals have been proposed by a number of authors (see Refs. [1–5, 15–17] and references therein). In the present work, we undertake to calculate in a novel manner the ultimate strength, brittleness parameter and their temperature dependence for crystal solids.

For this propose let us consider a configuration of atoms in a simple cubic crystal with a defect density low enough for the characteristic distance between dislocations to be large in comparison with the interatomic distance. The assumption that the relative arrangement of atoms in a given element is approximately the same than the arrangement of lattice sites, means that there can be a mutually one-to-one mapping of the atoms onto the lattice sites which conserves the neighborhood relation. The nearest neighbors of an atom correspond to those sites that are closer to its image on the lattice. The Hamiltonian of such a system, expressed with regard to the Frenkel-Kontorova dislocation model [18], may be written in the form[3]

$$\begin{aligned} H = (2m)^{-1} \sum_i \sum_k P_{ik}^2 + \sum_{i<j} \sum \sum_k U(\vec{r}_{ij}) \Big|_{\langle \vec{r}_{ij} \rangle_{k \neq 0}} \\ + \sum_{i<j} \sum \sum_{k \neq l} \frac{G}{4\pi^2} \frac{a_k^4}{\langle \vec{r}_{ij} \rangle_l} \left(1 - \cos \frac{2\pi r_k}{a_k}\right) \Big|_{\langle \vec{r}_{ij} \rangle_{k \neq 0}} , \end{aligned} \tag{1}$$

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[1] It was this observation that led to the development of dislocation theory in the 1930's.

[2] For example, under dynamic loading when kinetical processes of dislocation (and other defect) are not decisive in the response of irreversibly deformed solids [1, 6, 14].

[3] Notice that the common approximation (see, for example, Refs. [2, 3]) which takes into account only interactions between the nearest atoms in a crystal with a simple cubic structure leads to a zero shear modulus [19]. On the other hand, the common consideration of the sliding of atomic planes one over another (see [2, 4]) do not permit tensile strength calculations. The Frenkel-Kontorova dislocation model [18] used in Hamiltonian (1) makes it possible to eliminate these obstacles and consistently defines crystal behavior in shearing and tension. Notice that this is equivalent to selecting the suitable angle dependence of interatomic potential which is the function of interatomic distances (see Ref. [20]).

where $\vec{r}_i = \langle\vec{r}_i\rangle + \vec{u}_i$, $\vec{u}_i$ is the vector of displacement of the ith atom from its position of the thermal equilibrium $\langle\vec{r}_i\rangle$, $\vec{r}_{ij} = \vec{r}_i - \vec{r}_j$; a_k are the lattice constants, m is mass of an atom, and P_{ik} is the momentum conjugated with Cartesian coordinates (k) of the ith atom. The last (third) term in Eq. (1) represents the generalization of the three-dimensional case of contribution to the Hamiltonian from the "base" by the analogy with Frenkel-Kontorova model, which is stated in the potential form (r_k is the current linear coordinate "along the base").

Proceeding from the variational principle in statistical mechanics (see [21]) and the Gibbs-Bogolyubov inequality (see [22]) it is possible to calculate the free energy F of the crystal which obeys the Hamiltonian (1), by minimizing the right side of the expression

$$F \le F_m \equiv F_0 + \langle H - H_0\rangle, \tag{2}$$

where F_0 is the free energy of the model system with the Hamiltonian H_0; the mean values of $\langle\ldots\rangle$ are taken within the canonical ensemble characterized by the model Hamiltonian H_0.

Employing the self-consistent harmonic method [23], the thermodynamic properties of the system under consideration can be readily computed by using as the model system a set of harmonic oscillators (Einstein's model [21]) with variational force constants λ_i and lattice constant a_0. In the high-temperature approximation [22], when crystal atoms are exposed to external forces, the minimum of the free energy may be determined by self-consistent computation of the force constants λ_i and the equilibrium atom positions $\langle\vec{r}_i\rangle$. A pair interatomic Morse potential $U(\vec{r})$ [2] may be employed for dynamic properties of the linear atomic chain imposing the following condition

$$U''(r)\Big|_{r=a_k} = E_l a_k, \tag{3}$$

which leads to the following expression for the shear modulus G at the final temperature:[4]

$$G = \tfrac{1}{5}[(C_{11} - C_{12}) + 3\,C_{44}] = \frac{\langle U''(\langle\vec{r}_{ij}\rangle_l)\rangle}{\langle\vec{r}_{ij}\rangle_l}\,\frac{1-2\nu}{2(1-\nu)}. \tag{4}$$

Here E_l is the longitudinal modulus, C_{ij} are elastic constants, and ν is the Poisson's ratio.

To calculate the temperature dependence of the threshold tensile stress, let us consider a uniform tension of simple cubic lattice in the x-direction under stress σ_{11}. This results in increase of the distance between neighboring planes normal to direction of stress on the value u_x along the axis [100]. The threshold stress may be determined from the maximum of the function $u_x(\varepsilon)$ for each temperature in the self-consistent computation using following equations:

$$\sigma_{11} = 4\left(\frac{a_0}{a_T}\right)^2 \sigma_{\mathrm{C}}^0 \exp\left(-\frac{1}{4}\frac{\varepsilon a_T}{\varepsilon_{\mathrm{C}}^* a_0}\right)\left[1 - \exp\left(-\frac{1}{4}\frac{\varepsilon a_T}{\varepsilon_{\mathrm{C}}^* a_0}\right)\right]\exp\left(-\frac{T_a}{\Lambda_1}\right), \tag{5}$$

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[4] Averaging was performed by the Gauss method [21].

$$\Lambda_1(T) = \frac{2}{3}\exp\left(-\frac{T_a}{\Lambda_1(T)}\right)\left\{1+\frac{1-2\nu}{1-\nu}\times\exp\left[-32\pi^2\left(\frac{a_0}{a_T}\right)^2\frac{T_a}{\Lambda_1(T)}(\varepsilon_{\mathrm{C}}^*)^2\right]\right\}$$
$$\times\left[2\exp\left(-\frac{1}{2}\frac{\varepsilon a_T}{\varepsilon_C^* a_0}\right)-\exp\left(-\frac{1}{4}\frac{\varepsilon a_T}{\varepsilon_C^* a_0}\right)+2\right], \tag{6}$$

where

$$\varepsilon \equiv \frac{u_x}{a_T}, \qquad \varepsilon_{\mathrm{C}}^* \equiv \frac{\sigma_{\mathrm{C}}^0}{E_{\mathrm{l}}}, \qquad T_a \equiv k_{\mathrm{B}}\frac{T}{U_{\mathrm{b}}}, \qquad \Lambda_1(T) \equiv \frac{\lambda_1}{E_{\mathrm{l}} a_T}. \tag{7}$$

Here a_T and a_0 are the parameters of the elementary cell at temperature T and 0 K, respectively; k_{B} is the Boltzmann's constant; and U_{b} is the bond energy, which is related to the atomization energy (sublimation) of g-atom of solid H_0 as

$$U_{\mathrm{b}} = 2\frac{H_0}{N_{\mathrm{A}} n_{\mathrm{b}}}, \tag{8}$$

where n_{b} is the bonds number (nearest neighbors) about the elementary cell[5] and N_{A} is the Avogadro's number.

To calculate the temperature dependence of the shear ultimate strength,[6] let us consider a simple cubic lattice under the uniform shear stress τ_{12}, which governs a shear δ of the neighbor atomic planes of the {001} type. In this case the self-consistent system of constitutive equations takes the form

$$\tau_{12} = \tau_{\mathrm{C}}^0\frac{a_0}{a_T}\sin\left(2\pi\frac{\delta}{a_T}\right)\exp\left[-32\pi^2\left(\frac{a_0}{a_T}\right)\frac{T_a}{\Lambda_\tau(T)}(\varepsilon_{\mathrm{C}}^*)^2\right]\exp\left(-\frac{T_a}{\Lambda_\tau(T)}\right), \tag{9}$$

$$\Lambda_\tau(T) = \exp\left(-\frac{T_a}{\Lambda_\tau(T)}\right)$$
$$\times\left\{2+\frac{1-2\nu}{3(1-\nu)}\exp\left[-32\pi^2\left(\frac{a_0}{a_T}\right)^2\frac{T_a}{\Lambda_\tau(T)}(\varepsilon_{\mathrm{C}}^*)^2\right]\left[5+\cos\left(2\pi\frac{\delta}{a_T}\right)\right]\right\}. \tag{10}$$

It is easy to see that at $T = 0$ K Eqs. (5)–(8) and (9), (10) leads to the well known expressions (see, for example Refs. [1, 2]) for ultimate tensile and shear threshold stresses,

$$\sigma_{\mathrm{C}}^0 = \sqrt{\frac{n_{\mathrm{b}}}{144}H_0} \quad \text{and} \quad \tau_{\mathrm{C}}^0 = \frac{G}{2\pi}, \tag{11}$$

respectively.

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[5] The coefficient 2 in Eq. (8) results from the sum of all the energy of interatomic bonds, where each bond appears twice.

[6] The ultimate shear strength in original Frenkel-Kontorova model [18] is calculated considering the interaction of two parallel atomic linear chains.

It immediately follows from Eqs. (5), (6) and (9), (10) that the temperature dependences of the threshold stresses are governed only by two dimensionless parameters of the material under study, namely, by the Poisson's ratio ν[7] and effective critical value of elastic deformations $\varepsilon_{\mathrm{C}}^{*} = \sigma_{\mathrm{C}}^{0}/E_{\mathrm{l}}$.

The results of the computing of Eqs. (5), (6) and (9), (10) are convenient to present in the coordinates: *ultimate strength normalized to the longitudinal modulus* ($\sigma_{\mathrm{C}}/E_{\mathrm{l}}$ or $\tau_{\mathrm{C}}/E_{\mathrm{l}}$) and *the normalized temperature* (T/T_{C}), where T_{C} is the critical temperature crystal structural stability [1], which is governed by the equation

$$T_{\mathrm{C}} = 4\frac{U_{\mathrm{b}}}{k_{\mathrm{B}}} \max_{x} \left\{ x \exp(-2x) \left[1 + \frac{1-2\nu}{1-\nu} \exp\left(-32\frac{\pi^2}{y(x)} \right) \right] \right\}, \tag{12}$$

where $y(x) = \left[\left(\varepsilon_{\mathrm{C}}^{*}\sqrt{2x} \right)^{-1} + 6\sqrt{2x} \right]^{2}$.

The results of computing temperature dependence of tensile and shear threshold stresses by using Eqs. (5), (6) and (9), (10) have shown that there are three different types of relations between the functions $\sigma_{*}(T) = \sigma_{\mathrm{C}}/E_{\mathrm{l}}$ and $2\sqrt{2}\,\tau_{*} = 2\sqrt{2}\,\tau_{\mathrm{C}}/E_{\mathrm{l}}$, which are presented in Figs. 1a–c. Recalling that when $\sigma_{\mathrm{C}} < 2\sqrt{2}\,\tau_{\mathrm{C}}$ the crystal is brittle, and if $\sigma_{\mathrm{C}} > 2\sqrt{2}\,\tau_{\mathrm{C}}$ it is ductile [1, 5]. Thus, the transition from the brittle to the ductile state of a crystal solid may be determined by the condition

$$\sigma_{\mathrm{C}}(T_{*}) = 2\sqrt{2}\,\tau_{\mathrm{C}}(T_{*}). \tag{13}$$

Hence, graphs in Fig. 1a are associated with the truly brittle crystal; graphs in Fig. 1b are associated with a ductile crystal; while a crystal which is characterized by third type of the ($\sigma_{\mathrm{C}}/\tau_{\mathrm{C}}$)–diagram (Fig. 1c) can be treated as a quasi-brittle or quasi-ductile material.

The specific relations between the parameters ν and $\varepsilon_{\mathrm{C}}^{*}$ corresponding to these three types of materials are presented in Fig. 1d. The last diagram evaluates the character of material fracture according to an adiabatic model under consideration. These results give rise to suggest a physical criterion of brittleness. We define the brittleness parameter as the renormalized value of the effective critical elastic deformation, namely,

$$B_{*} = \frac{\varepsilon_{\mathrm{C}}^{*}}{\varepsilon_{\mathrm{C}}^{0}}, \tag{14}$$

where $\varepsilon_{\mathrm{C}}^{0}$ is governed by the condition $\sigma_{\mathrm{C}}^{0} = 2\sqrt{2}\tau_{\mathrm{C}}^{0}$ and thus (see Eqs. (11)) is equal to the ratio H_0/E_{l}.

Now, it is straightforward to see that the crystal is truly brittle if $B_{*} < 0.63 \div 0.67$, and it is ductile if $B_{*} \geq 1$. Quasi-brittle and quasi-ductile materials are characterized by a brittleness parameter within the interval $0.65 < B_{*} < 1$.

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[7] Theoretical methods for the calculation ν and its temperature dependence are considered in [24, 24].

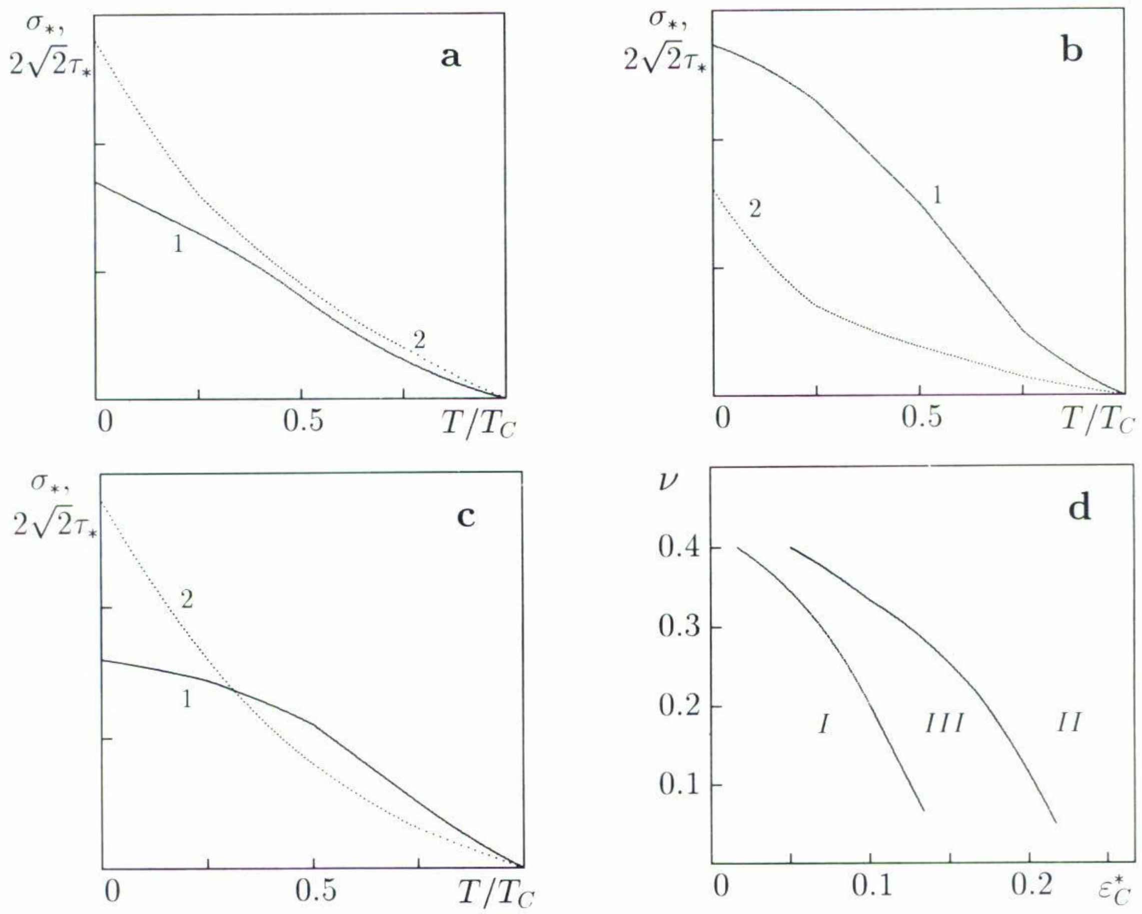

FIGURE 1. Temperature dependence of ultimate tensile (1) and shear (2) strength for brittle (a), ductile (b), and quasi-brittle or quasi-ductile (c) materials and the diagram of the fracture character by adiabatic model: *I*: brittle cleavage, *II*: ductile fracture, and *III*: there is the brittle-ductile transition.

As we can see from the data listed in Table I,[8] the results of brittleness estimation by means of suggested parameter B are in a good agreement with results based on the brittleness parameter $Re_{cr} = H_0/G$ suggested in Ref. [26] within a framework of quantum-statistical approach to dynamic problems of solid mechanics (see also review [14]), as well as with the results obtained using brittleness numbers $\eta = \sqrt{Gb/\gamma}$[9] and $\eta_{\mathrm{b}} = \sqrt{b\tau_0/\gamma}$[10] which were suggested within a framework of different dislocation models of quasistatic ductile fracture by Rice and Thomson [7] and Cherepanov [8], respectively.

The merit of the brittleness parameter B_* over the brittleness numbers η and η_{b} is that

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[8] Parameters for materials with complex crystal structure were calculated using the effective cell concept [1, 14].

[9] b is the Burgers vector absolute value of the elementary dislocation, and γ is the surface tension (density of the surface energy).

[10] τ_0 is the friction (Shmid) force.

TABLE I. Ultimate tensile strength and various brittleness parameters for some crystal materials.

Material	σ_C, GPa	B_*, Eq. (14)	Re_{cr} [1,14]	η_b^{-1} [8,27]	η^{-1} [7]
Ductile materials, $B_* \geq 1$ ($Re_{cr} > 0.707$ [26], $\eta_b^{-1} \gg 1$ [8], $\eta^{-1} \geq 0.35$ [7]).*					
Au	25.3	1.81	1.01	70	0.45
Al	18.5	1.44	1.14	$25 \div 50$	0.35
Ag	18.9	1.28	0.85	$50 \div 100$	0.39
Ti	24.6	1.26	1.10	40	?
Cu	29.0	1.18	0.93	$30 \div 50$	0.40
Quasi-ductile and quasi-brittle materials, $0.65 < B_* < 1$ ($\eta_b^{-1} \sim 1$ [8]).					
Fe	38.1	0.90	0.71	10	0.34
Ru	57.2	0.73	0.70	?	?
Mo	40.9	0.72	0.61	0.87	?
W	50.5	0.70	0.55	0.93	0.33
Al_2O_3	49.8	0.68	0.705	0.63	0.24
Brittle materials, $B_* < 0.65$ ($Re_{cr} < 0.707$ [27], $\eta_b^{-1} < 1$ [8], $\eta^{-1} < 0.25$ [7]).					
B_4C	48.2	0.53	0.60	?	?
Si	13.9	0.46	0.52	0.77	0.23
Ge	10.7	0.42	0.53	?	0.18
SiC	37.1	0.41	0.32	0.59	?
Diamond	81.7	0.34	0.51	0.42	0.20

* Notice the difference in the condition of ductility according to different criteria.

for the calculation of the first one, one needs only data for elastic moduli and atomization (sublimation) energy, which in contrast to the data for γ and τ_0 are well defined.[11]

Thus, using the suggested model we can predict the nature of a given crystal material (brittle, quasi-brittle, ductile, quasi-ductile) and estimate its ultimate tensile and shear strength.[12]

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[11] It should be emphasized, that elastic properties and sublimation energy of solid materials can be estimated more accurately than the surface tension and friction force. In fact, data variation for the last material constants reaches 100–300% [2,3] and there is little data for temperature dependence of γ (we do not know the data for temperature dependence of τ_0).

[12] Notice that ultimate tensile strength should be equal to the Griffith strength [2,3] and we can use Eqs. (5), (11) for estimation of the surface tension γ, while the ultimate shear strength (9), (11) may be observed only for a certain conditions of dynamic loading (see Ref. [14]).

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