Modeling of the temperature-dependent ideal shear strength of solid single crystals

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ABSTRACT

Knowledge of the ideal shear strength of solid single crystals at finite temperatures is of fundamental importance. It is mainly determined by the molecular dynamics simulations. However, thus obtained results are strongly dependent on the employed empirical potentials. In the present work, two theoretical models for the temperature-dependent ideal shear strength of single crystals are established based on the Frenkel's classical theory and the energy view. To test the established models, the ideal shear strengths of β-NiAl and γ-Ni$_3$Al alloys are calculated from 0 K to the melting point and compared with the results reported in the literature. The study shows that both shear modulus and ideal shear strength firstly remain approximately constant and then decrease almost linearly as temperature changes from 0 K to melting point. However, the ideal shear strength has stronger temperature dependence than the shear modulus.

1. Introduction

The ideal shear strength of solids is the upper bound of the shear stress that the material can attain during shear. It is solely determined by the nature of the atomic bonding of the material and is a function of temperature. Its knowledge is important to a wide range of material behaviors, such as the elastic instability (or phonon softening) of single crystals, nucleation of dislocation, and formation of stacking fault [1,2].

The first well-known estimation for the ideal shear strength of solids is due to Frenkel [3] (see Eq. (4)). In his calculations, just the first term of the Fourier series for the potential energy was considered [4]. The existing studies show that this equation often overestimates the ideal shear strength of solids [5]. Later, Mackenzie [6] attempted to take further terms into consideration. Unfortunately, the ideal shear strength was not presented explicitly and one uncertain critical parameter was involved. This makes it almost impossible to use.

At present, the most accurate method to calculate the ideal shear strength of solids is the *ab initio* (AI) (or first principles) calculations [2,7–10], in which only some basic structural information is needed. However, this method is mainly limited to 0 K and it is still a challenge to treat finite temperatures [11–14]. Approximation methods (mainly referring to the molecular dynamics (MD) simulations) have thus been used to predict the ideal shear strength of single crystals at finite temperatures [2,15–17]. However, as well known, the results given by

these methods are strongly dependent on the employed empirical potentials [11–14]. They can overestimate the ideal shear strength at high temperatures (as shown in this work; see Fig. 2(b)).

In the present work, two theoretical models for the temperature-dependent ideal shear strength of solid single crystals are established. One is based on the Frenkel's classical theory. The other is in the view of energy. To test the established models, the ideal shear strengths of β-NiAl and γ-Ni$_3$Al alloys are calculated from 0 K to the melting point and compared with the results reported in the literature. The temperature dependence of the ideal shear strength is discussed.

2. Theoretical models

2.1. Model based on Frenkel's idea

Consider a crystal that has a periodical structure in which the repeat distance in the direction of shear is b and that perpendicular to the shear direction is a. Assume that the energy-displacement curve during shear deformation is a sine form. The shear stress can then be expressed as:

$$\tau = \tau_c \sin\left(\frac{2\pi x}{b}\right) \tag{1}$$

where τ_c is the peak stress of the sine function, i.e., the ideal shear

strength; x is the shear displacement; and π is the circumference ratio. For small displacement, Eq. (1) can be written as:

$$\tau = \tau_c \frac{2\pi x}{b} \tag{2}$$

In addition, the shear stress τ can also be expressed as:

$$\tau = G\gamma \tag{3}$$

where $\gamma = \frac{x}{a}$ is the shear strain and G is the shear modulus. Let Eq. (3) to be equal to Eq. (2) one obtains:

$$\tau_c = \frac{Gb}{2\pi a} \tag{4}$$

Equation (4) is the well-known Frenkel's model [3].

Note that in Eq. (4) all the parameters are temperature-dependent. If the ideal shear strength of the material at the reference temperature T_0 is known, from Eq. (4), one obtains:

$$\tau_c(T_0) = \frac{G(T_0)b(T_0)}{2\pi a(T_0)} \tag{5}$$

Combining Eq. (5) with Eq. (4) one obtains:

$$\tau_c(T) = \tau_c(T_0)\frac{G(T)}{G(T_0)}\frac{b(T)a(T_0)}{b(T_0)a(T)} \tag{6}$$

For convenience, the reference temperatures of the coefficients of the linear thermal expansion along a and b can be chosen as T_0. Thus, the following equations hold:

$$a(T) = a(T_0)[1 + \alpha(T)(T - T_0)] \tag{7a}$$

$$b(T) = b(T_0)[1 + \beta(T)(T - T_0)] \tag{7b}$$

where α and β are the coefficients of the linear thermal expansion along a and b, respectively. Equation (6) can then be rewritten as:

$$\tau_c(T) = \tau_c(T_0)\frac{G(T)}{G(T_0)}\frac{1 + \beta(T)(T - T_0)}{1 + \alpha(T)(T - T_0)} \tag{8}$$

2.2. Model based on energy view

According to the classical theory for shear deformation of crystals, in the above problem, the shear stress τ changes with the shear displacement x as a sine function and becomes zero first at $x = \frac{1}{2}b$. The work required to complete this process is the unstable stacking fault energy and can be expressed as [1]:

$$\gamma_{us} = \frac{8aG\gamma_c^2}{\pi^2} \tag{9}$$

where $\gamma_c = \frac{1}{4a}b$ is the ideal shear strain. From Ogata et al.'s [5] study, the following equation holds:

$$\tau_c = \frac{kG\gamma_c}{\pi} \tag{10}$$

where k is a material constant. Besides, according to Iskandarov et al. [16], k is almost temperature-independent. Thus, Eq. (9) can be re-expressed as:

$$\gamma_{us} = \frac{8a\tau_c^2}{k^2G} \tag{11}$$

It is known that the unstable stacking fault energy of single crystals decreases as temperature increases. The increase or decrease of quantity of heat of the material is the gain or loss of phonon which results in the change of temperature and can be quantified by using the specific heat. The heat energy increase when temperature changes from T_0 to T can be calculated by integrating the specific heat at constant pressure C_p over this temperature range. Given that the unstable stacking fault energy γ_{us} at the reference temperature T_0 is known. Thus, for simplicity, γ_{us} can be expressed as:

$$\gamma_{us}(T) = \gamma_{us}(T_0) - K\int_{T_0}^{T} C_p(T)\mathrm{d}T \tag{12}$$

where K is the coefficient characterizing the reduction of the unstable stacking fault energy with increasing temperature. Besides, K can also be considered as a transfer coefficient between the heat energy and the unstable stacking fault energy, similar to that shown in Cheng et al. [11,12]. In addition, for single crystals, the material can still resist deformation approaching the melting point [11,12] and will become liquid after absorbing heat energy of ΔH_M (melting heat) at the melting point T_m and thus loses the ability to resist shear deformation. Thus, applying Eq. (12) at the melting point, K can be determined as:

$$K = \frac{\gamma_{us}(T_0)}{\int_{T_0}^{T_m} C_p(T)\mathrm{d}T + \Delta H_M} \tag{13}$$

Substituting Eq. (13) into Eq. (12), one obtains:

$$\gamma_{us}(T) = \gamma_{us}(T_0)\left[1 - \frac{1}{\int_{T_0}^{T_m} C_p(T)\mathrm{d}T + \Delta H_M}\int_{T_0}^{T} C_p(T)\mathrm{d}T\right] \tag{14}$$

As shown earlier, Eq. (11) holds at any temperature. In particular, at the reference temperature, Eq. (11) becomes:

$$\gamma_{us}(T_0) = \frac{8a(T_0)(\tau_c(T_0))^2}{k^2G(T_0)} \tag{15}$$

From Eqs. (11) and (15),

$$\frac{\gamma_{us}(T)}{\gamma_{us}(T_0)} = \frac{a(T)(\tau_c(T))^2G(T_0)}{a(T_0)(\tau_c(T_0))^2G(T)} \tag{16}$$

Note that the parameter k has been reduced during the derivation because of its temperature independence. According to the definition of the coefficient of the linear thermal expansion (Eq. (7)), Eq. (16) can be further expressed as:

$$\frac{\gamma_{us}(T)}{\gamma_{us}(T_0)} = \frac{(1 + \alpha(T)(T - T_0))(\tau_c(T))^2G(T_0)}{(\tau_c(T_0))^2G(T)} \tag{17}$$

From Eqs. (14) and (17), the ideal shear strength can be expressed as:

$$\tau_c(T) = \tau_c(T_0)\left\{\frac{1}{1 + \alpha(T)(T - T_0)}\frac{1}{G(T_0)}G(T)\right.$$

$$\left.\times\left[1 - \frac{1}{\int_{T_0}^{T_m} C_p(T)\mathrm{d}T + \Delta H_M}\int_{T_0}^{T} C_p(T)\mathrm{d}T\right]\right\}^{\frac{1}{2}} \tag{18}$$

2.3. Discussion on the models

Hereto, two temperature-dependent theoretical models for the ideal shear strength of single crystals have been established. One can see that the model based on Frenkel's idea (Eq. (8)) relates the temperature dependence of the ideal shear strength to that of the coefficients of the linear thermal expansion and shear modulus. The model based on energy view (Eq. (18)) relates the temperature dependence of the ideal shear strength to that of the coefficient of the linear thermal expansion, shear modulus, and the specific heat at constant pressure of materials. The ideal shear strength at the reference temperature can be calculated using the AI method. The temperature-dependent coefficients of the linear thermal expansion, shear modulus, and specific heat at constant pressure, as well as the melting point and melting heat, can be found in the literature and materials handbooks. Thus, the theoretical models can be applied conveniently. Note that phase transition is not considered above. For that case, the heat of phase transition should also be included in the equations; see Cheng et al. [11–14].