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Relation of flow stress to the mean-square amplitude of atomic vibrations in cubic metals

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The critical resolved shear stress (CRSS) of 14 face-centered- and body-centered-cubic elements in the temperature range 0 to 300 K has been examined as a function of the mean-square amplitude of atomic vibration $\langle u^2 \rangle$ measured at room temperature. It is found that the CRSS of elements with a given crystal structure is a unique function of $\langle u^2 \rangle$. For a given temperature and crystal structure, the CRSS decreases as $\langle u^2 \rangle$ increases. The dislocation lines composed of atoms with large $\langle u^2 \rangle$ value have low line tension, and are easy to move in the slip plane of the crystal, resulting in a low CRSS value.

INTRODUCTION

The glide of dislocations results in slip, which is the most common manifestation of plastic deformation in crystalline solids. A characteristic tensile or compressive stress is required to start slip in crystals; the component of this applied stress, resolved on the slip plane in the slip direction, is called the critical resolved shear stress (CRSS). It is well established that the CRSS for slip in metals depends on a number of factors, namely, crystal structure, dislocation density, orientation of single crystals, grain size of polycrystals, elemental purity, strain rate, and temperature at which crystal is deformed, and heat-treatment prior to deformation, etc. Abundant data on the CRSS of metallic crystals as a function of these parameters are available in the literature,[1-20] and several attempts have been made in the past to explain the observations in terms of sophisticated dislocation theories.[21-25] Recent investigations carried out by Butt, Bashir, and Khan[26] on the interrelation between the micro and the macro aspects of cubic elements have, however, set new trends in the interpretation of the physical and mechani-

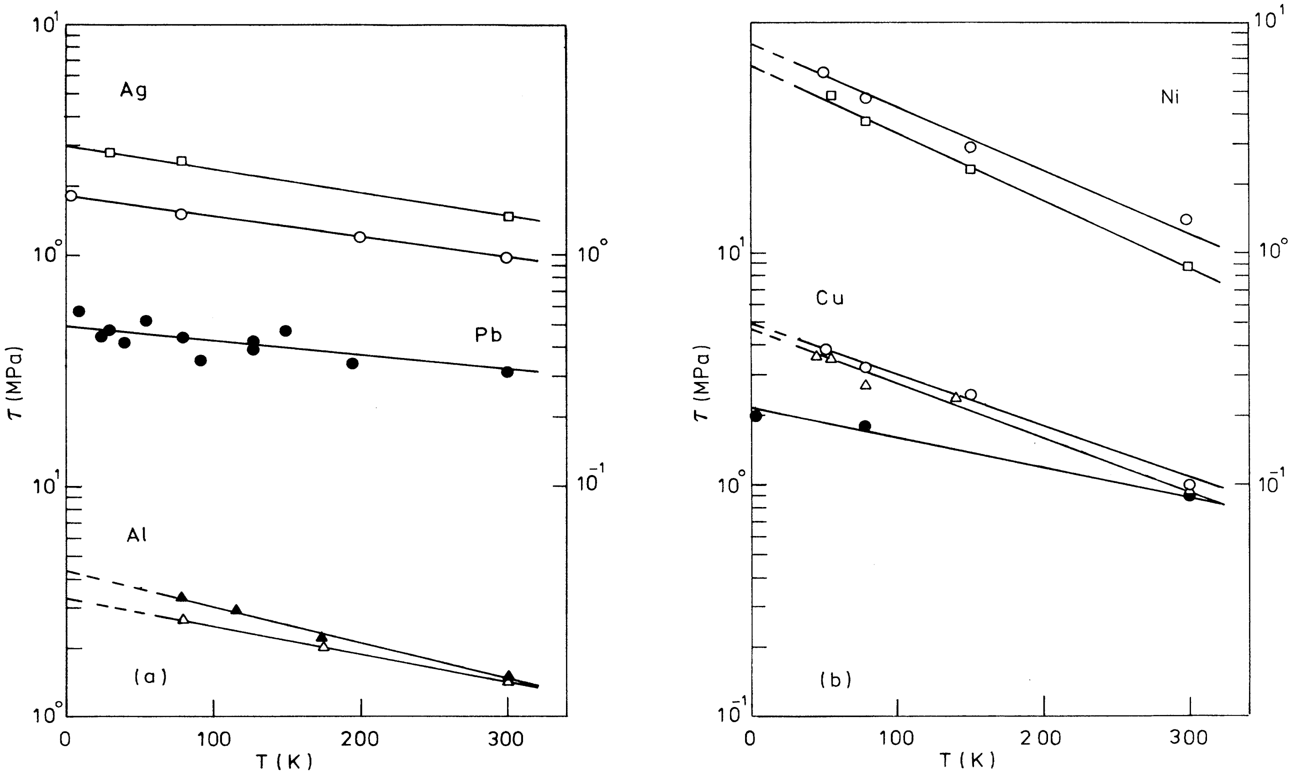

FIG. 1. Semi-logarithmic representation of the temperature dependence of the CRSS for (a) single crystals of Ag[1] (□ 99.99%, $\dot{\epsilon}=7\times10^{-4}\ \mathrm{s}^{-1}$), Ag[2] (○ 99.99%, $\dot{\epsilon}=10^{-4}\ \mathrm{s}^{-1}$), 99.999% Pb[3] (●), and Al[4] (▲ 99.99%, △ 99.997%, $\dot{\epsilon}=7\times10^{-4}\ \mathrm{s}^{-1}$). (b) Polycrystalline Ni[5] (○ 99.998%, □ 99.999%, grain size = 180 μm, $\dot{\epsilon}=10^{-5}\ \mathrm{s}^{-1}$), Cu[6] single crystal (● 99.996%, $\dot{\epsilon}=6\times10^{-4}\ \mathrm{s}^{-1}$), and polycrystals of Cu[7] (○ 99.999%, grain size = 130 μm, $\dot{\epsilon}=1.3\times10^{-3}\ \mathrm{s}^{-1}$) and Cu[5] (△ 99.99%, grain size 75 μm, $\dot{\epsilon}=10^{-5}\ \mathrm{s}^{-1}$).

cal properties of crystalline materials. For instance, the excellent correlations observed by Butt, Bashir, and Kahn[26] between the elastic constants C_{11}, C_{12}, and C_{44} and the mean-square amplitude of atomic vibrations seems to have implications for the deformation behavior of cubic crystals beyond the elastic limit as well. This motivated the present study to explore the possibility of correlating the macroscopic CRSS of cubic metals with a single microscopic parameter: the amplitude of atomic vibrations.

The mean-square amplitude of atomic vibrations $\langle u^2 \rangle$ is a fundamental parameter of a crystal at a given temperature. The intensity of radiations (x rays, neutrons, γ rays, and electrons) diffracted from a crystal depends on $\langle u^2 \rangle$, and its variation with temperature has been extensively dealt with using the Debye-Waller theory.[27,28] With the rise of temperature, $\langle u^2 \rangle$ increases and the intensity of diffracted radiations decreases by an exponential factor known as the Debye-Waller factor, $\exp(-2B \sin^2\theta/\lambda^2)$, where θ is the Bragg angle at which the diffracted intensity is measured and λ is the wavelength of the radiation. The quantity B is usually referred to as the Debye-Waller thermal parameter or temperature factor. For a monoatomic cubic crystal for which the vibrations are isotropic, $B=8\pi^2\langle u^2 \rangle/3$. In 1988 Butt *et al.*[29] recommended the most accurate values of B factor at room temperature for 22 cubic elements. Using this data we shall investigate the correlation of the microscopic Debye-Waller thermal parameter B with the macroscopic CRSS of various face-centred-cubic (fcc) and body-centred-cubic (bcc) metals, as well as that for the line energy per unit length or line tension of the dislocations in cubic crystals.

RELATION BETWEEN CRSS AND *B* FACTOR

The points in Figs. 1–3 depict the CRSS data as a function of temperature in log/linear coordinates for 14 fcc (Ag[1,2], Pb[3], Al[4], Ni[5], and Cu[6,7]) and bcc (K[8,11], Li[9,11] Na[10,11], V[12], Mo[13], Ta[14,15], Nb[15], Fe[16–18], and W[19]) metal crystals of different orientations, grain sizes, purities, etc., deformed at various strain rates in the temperature range 4–300 K. The details of various parameters referred to above are given in the captions to the figures. It is noteworthy that a Taylor factor of $\frac{1}{3}$ was used to get the CRSS values τ from the available tensile yield stress σ (i.e., $\sigma=3\tau$) in the case of polycrystals. A linear relationship between $\log \tau$ and temperature T is evident. On extrapolating the line drawn through the $\log \tau/T$ data points for a given crystal to $T \rightarrow 0$ K, the intercept made on the stress axis gives a measure of the CRSS τ_0 at $T \rightarrow 0$ K. The thermal behavior of the CRSS of a given element can be quantified by a parameter, termed as fractional thermal softening (FTS) factor$=-(1/\tau_0)(d \ln \tau/dT)$, which not only specifies the rate of CRSS variation with temperature (i.e., $d \ln \tau/dT$) but also the exact position of the $\log \tau/T$ line on the semilogarithmic τ/T diagram.

Now we shall examine the dependence of the CRSS τ_{298}, τ_{200}, τ_{78}, and τ_0 pertaining to 298, 200, 78, and 0 K, respectively, as well as that of the FTS factor on the Deybe-Waller thermal parameter B (room temperature) for 14 cubic elements referred to above. The points in Fig. 4 represent the CRSS data for 0, 78, 200, and 298 K as a function of the B factor in double-logarithmic coordinates for Ni, Cu, Ag, Al, and Pb (fcc) as well as for W, Ta, Mo, Fe, Nb, V, Li, Na, and K (bcc) crystals. Similar-

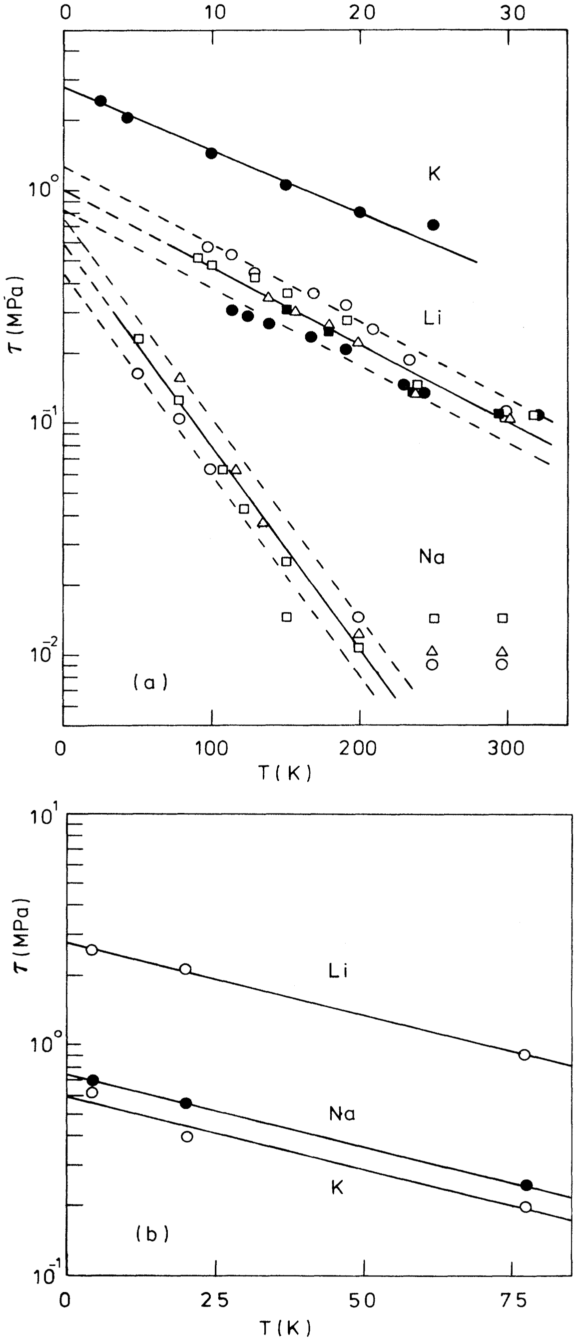

FIG. 2. The τ/T data depicted in log/linear coordinates for (a) single crystals of 99.99% K,[8] 99.999% Li,[9] and 99.999% Na (Ref. 10) deformed at a strain rate of the order of 10^{-4} s^{-1}. For Na and Li, various symbols stand for different orientations; the temperature scale given at the top is for K. (b) Coarse grain (>1 mm) polycrystalline 99.999% K,[11] 99.7% Li,[11] and 99.998% Na (Ref. 11) deformed at $\dot{\epsilon}=1.1\times10^{-4}$ s^{-1}.

ly, Fig. 5 shows the dependence of the FTS factor on the B parameter for fcc and bcc elements. In each case, the line drawn through the data points for a given crystal structure by least-squares fitting is given by $\ln Y = \ln Y_0 + M_0 \ln B$ or by the power law $Y = Y_0 B^{M_0}$, where Y stands for the mechanical property, i.e., CRSS or FTS factor, and Y_0 and M_0 are numerical constants. The values of these constants, which are found to be sensitive to crystal structure and temperature, are given in Table I. Thus for a given crystal structure and temperature, the CRSS of cubic elements is basically a function of the mean-square amplitude of atomic vibrations $\langle u^2 \rangle$.

RELATION BETWEEN LINE TENSION AND B FACTOR

The line tension of dislocations in a crystal is an important parameter of strength and plasticity of crystalline materials. It is defined as the increase in energy per unit increase in the length of a dislocation line, and is given by $E = \frac{1}{2} G b^2$, where G is the shear modulus and b is the lattice parameter. The values of line tension E for 14 fcc and bcc metal crsytals have been denoted by points in Fig. 6 as a function of the Debye-Waller thermal parameter B (room temperature) in log/log coordinates. The straight line drawn through the data points by the least-

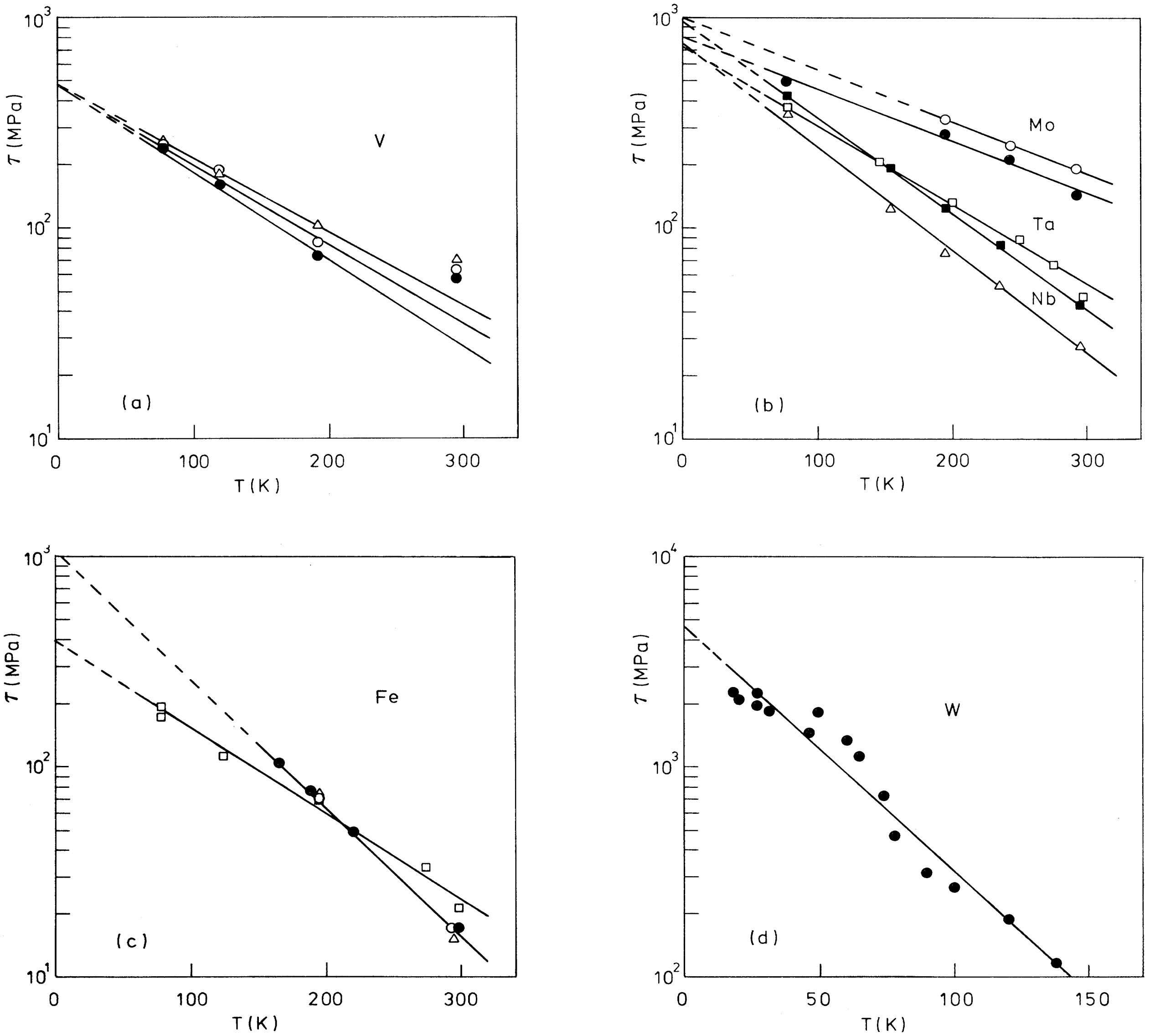

FIG. 3. Semilogarithmic representation of the τ/T data for (a) 99.9% V (Ref. 12) polycrystals of grain size 0.1 mm, deformed at strain rate $\dot{\epsilon}$: △ 3.3×10^{-2} s^{-1}, ○ 1.3×10^{-3} s^{-1}, and ● 3.3×10^{-5} s^{-1}. (b) High-purity single crystals of Mo (Ref. 13) (○ $\dot{\epsilon}=4.5\times10^{-3}$ s^{-1}, ● $\dot{\epsilon}=4.5\times10^{-5}$ s^{-1}), Ta (Ref. 14) (□ $\dot{\epsilon}=6\times10^{-4}$ s^{-1}), Ta (Ref. 15) (■ $\dot{\epsilon}=1.3\times10^{-4}$ s^{-1}), and Nb (Ref. 15) (△ $\dot{\epsilon}=1.3\times10^{-4}$ s^{-1}). (c) Zone refined single crystals of Fe (Ref. 16) (□ 99.999%, $\dot{\epsilon}=1.7\times10^{-4}$ s^{-1}), Fe (Ref. 17) (● 99.98%, $\dot{\epsilon}=1.7\times10^{-4}$ s^{-1}), Fe (Ref. 18) (△ 99.98%, $\dot{\epsilon}=3.3\times10^{-4}$ s^{-1}), and polycrystalline Fe (Ref. 18) (○ 99.98%, grain size = 65 μm, $\dot{\epsilon}=3.3\times10^{-4}$ s^{-1}). (d) Single-pass zone-refined 99.99% W (Ref. 19) single crystal.

squares-fit method is encompassed by the relation $\ln E = -24.80 - 0.88 \ln B$, irrespective of the type of crystal structure. Thus dislocation lines in crystals of elements with a large mean-square amplitude of atomic vibrations $\langle u^2 \rangle$ have low line tension, and vice versa.

INTERPRETATION OF EMPIRICAL CORRELATIONS

According to the kink-pair nucleation (KPN) model[7,25] of plastic flow, which will be discussed later, the CRSS of metallic crystals should vary with temperature as given

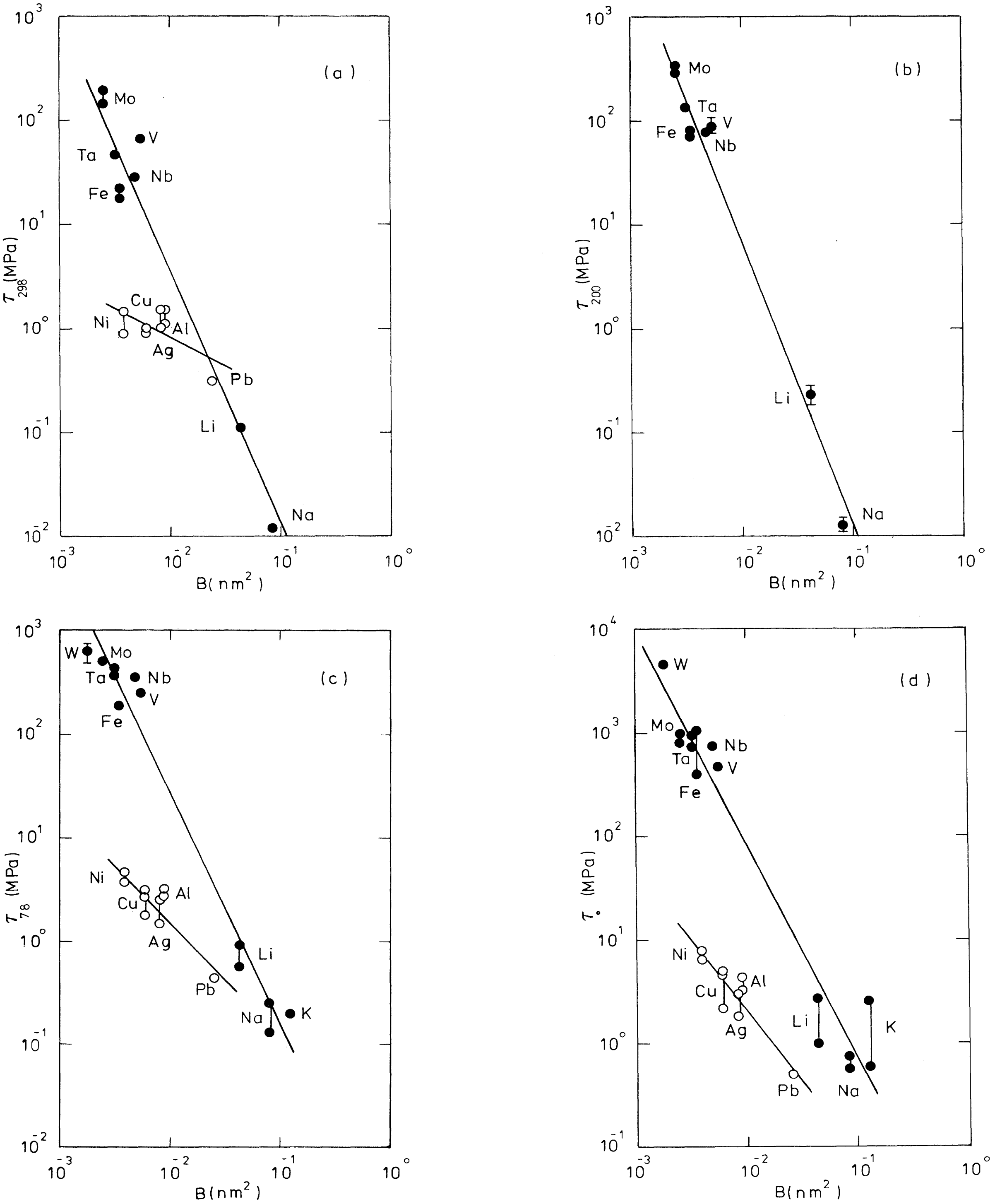

FIG. 4. The CRSS τ as a function of B factor (room temperature) for various fcc and bcc metals at (a) 298, (b) 200, (c) 78, and (d) 0 K. The points represent CRSS values given in Figs. 1–3, except the lower one for Al (Ref. 20) single crystal (99.999%, (1 1 11), $\dot{\gamma} = 1.6 \times 10^{-3}\ \mathrm{s}^{-1}$).

TABLE I. Values of constant $\ln Y_0$ and slope M_0 in the equation of straight line $\ln Y=\ln Y_0+M_0\ln B$ fitted to the data points in the plots of Debye-Waller thermal parameter B (nm^2) vs mechanical parameter Y (CRSS or FTS factor) in Figs. 4 and 5.

Mechanical parameter Y	fcc $\ln Y_0$	fcc M_0	bcc $\ln Y_0$	bcc M_0
τ_0 (MPa)	-5.75	-1.38	-5.19	-2.07
τ_{78} (MPa)	-4.51	-1.07	-7.16	-2.27
τ_{200} (MPa)	...	...	-10.64	-2.72
τ_{298} (MPa)	-2.70	-0.54	-10.15	-2.46
FTS (MPa^{-1} K^{-1})	-3.91	$+0.59$	$+1.57$	$+2.27$

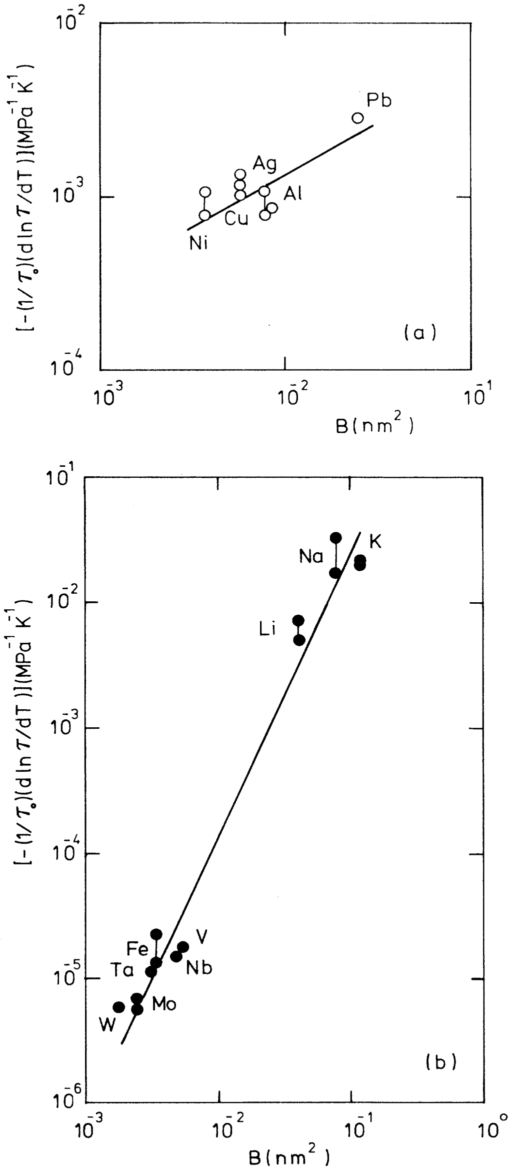

FIG. 5. The fractional thermal softening (FTS) parameter as a function of B factor (room temperature) for (a) fcc and (b) bcc metals.

by the relation

$$\tau=\tau_0\exp(-mkT/W_0)\ , \tag{1}$$

where τ is the CRSS at temperature T, $\tau\rightarrow\tau_0$ as $T\rightarrow0$ K, k is the Boltzmann constant, $m=25\pm2.3$ and W_0 is a positive constant specific to the material. Equation (1) is, however, valid at rather low temperatures only where diffusional recovery processes in the crystal do not occur, and it implies a linear temperature dependence of the logarithm of the CRSS. This is confirmed by experiment, as is evident from Figs. 1–3.

Concerning the relationship between the CRSS (0, 78, 200, and 298 K) and the B factor (room temperature) for various fcc and bcc metals referred to in Fig. 4, it must be pointed out that the values of CRSS pertaining to 0, 78, and 200 K were also correlated with the room-temperature B factor because reliable measured values of the B factor for most of these elements at rather low temperatures, like those available[29] at room temperature, are scant. However, we know that the mean-square amplitude of atomic vibrations is a function of temperature, and its value decreases as temperature is lowered. Thus on plotting the CRSS data obtained at a given temperature T below room temperature against the B factor for the corresponding temperature (if available), the functional form of the $\tau(T)/B(T)$ dependence would be expected to be similar to that depicted in Figs. 4(b)–4(d), except that the data points will then shift to the left along the B axis by an amount depending on the temperature T. Referring to Fig. 5, the excellent correlation between the FTS factor and the room-temperature B factor for various cubic elements of a given crystal structure indicates that the temperature dependence of the CRSS between 0 and 300 K is also a unique function of the mean-square amplitude of atomic vibrations at room temperature. It

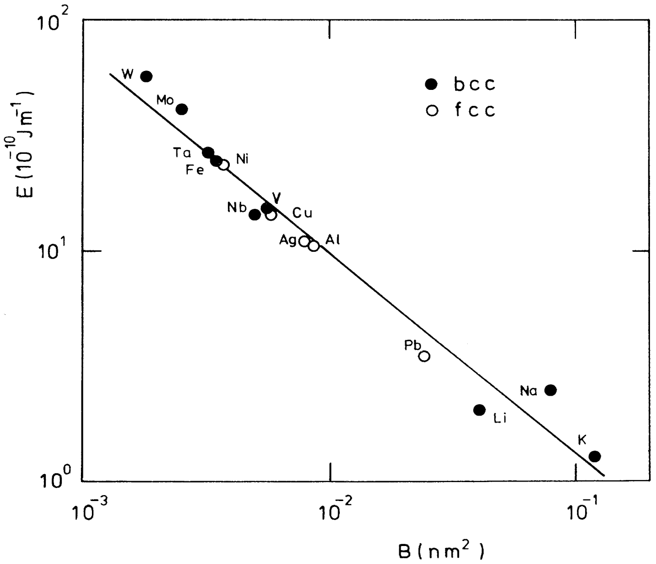

FIG. 6. The line energy per unit length or line tension E of dislocations in fcc and bcc metallic crystals versus B factor at room temperature.

is noteworthy that, although somewhat outside the scope of the present work, Butt, Bashir, and Khan[26] found that the melting point of cubic elements is also closely related to their room-temperature B factor.

To elaborate the effect of the mean-square amplitude of atomic vibrations on the CRSS of cubic elements, we shall have recourse to the KPN model[7,25] of plastic flow in metallic crystals. In this model, yielding of bcc metals[25] with high intrinsic lattice friction is visualized to occur as a consequence of stress-assisted, thermally activated, nucleation of a kink pair in the screw dislocation segment trapped in a Peierls valley, leading to its forward movement over the Peierls hill to the next valley, after attainment of the saddle-point configuration. At a given temperature, the dislocation line composed of atoms with a higher mean-square amplitude of atomic vibrations $\langle u^2 \rangle$ and thus having greater flexibility or lower line tension E (Fig. 6), will therefore find it easier to escape from the Peierls valley to nucleate slip at rather lower applied stress. Now, as the temperature of a given element is lowered, the $\langle u^2 \rangle$ value decreases, line tension E increases, and, consequently, the escape of the trapped dislocation segment from the Peierls valley by kink-pair nucleation will be possible only at higher applied stresses. This accounts for the observed increase in CRSS of bcc metals with a decrease in temperature (Figs. 2 and 3).

In the case of fcc metals with low intrinsic lattice friction, the unit activation process of yielding[7] comprises a stress-assisted, thermally activated breakaway of an edge dislocation segment from an array of pinning points, e.g., solid and gaseous impurities, forest dislocations, etc., by cooperative unzipping, and at the same time expanding in length sufficiently to facilitate the nucleation of a shallow arc, in a manner somewhat similar to the "kink-pair mode of escape" of screw dislocations from a Peierls barrier in bcc metals. Again a more flexible dislocation line composed of atoms with a higher mean-square amplitude of atomic vibrations $\langle u^2 \rangle$ at a given temperature will be able to detach itself from the anchoring points, and expand in length to attain a saddle-point configuration at rather lower applied stress, and vice versa. The observed increase in CRSS of fcc metals with decrease in temperature (Fig. 1) can also be explained by a reasoning similar to one given earlier for bcc metals.

CONCLUSIONS

The foregoing evidence leads us to the following conclusions.

(1) The mean-square amplitude of atomic vibrations $\langle u^2 \rangle$ is the most significant parameter which determines the CRSS of cubic elements of a given crystal structure.

(2) For a given temperature and crystal structure, the elements with smaller values of $\langle u^2 \rangle$ have larger CRSS values, and vice versa.

(3) The FTS factor $[-(1/\tau_0)(d \ln \tau/dT)]$ for elements of a given crystal structure is also high for high $\langle u^2 \rangle$ values.

(4) The dislocation lines composed of atoms with large $\langle u^2 \rangle$ have low line tension, irrespective of the type of crystal structure.

(5) The dislocation lines having low line tension or large $\langle u^2 \rangle$ values are easy to move in the slip plane of the crystal of a given structure, resulting in low CRSS.

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