8.7 A SEMI-PHENOMENOLOGICAL MODEL FOR DISLOCATION MOBILITY IN TUNGSTEN

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OBJECTIVE

The dependence of dislocation velocity in tungsten on the applied stress and temperature is investigated. First, we give a brief theoretical overview of the mechanisms of kink pair formation and the relationship to dislocation motion under stress. We then discuss the theory of phonon scattering and its influence on damping dislocations that move at stresses higher than values where kink motion controls dislocation mobility. A general phenomenological framework is presented, where semi-empirical equations for the dislocation velocity in tungsten are presented. The objective of this effort is to develop a more general procedure for dislocation velocity in other BCC, FCC and HCP metals on the basis of the phenomenological theory, supported by data collected from experiments and MD simulations.

SUMMARY

Dislocation mobility is a fundamental property of a material that determines many of the characteristics of plastic deformation. It is an essential ingredient in large-scale dislocation dynamics (DD) simulations, as it controls the rates of dislocation-dislocation interaction mechanisms, and thus the way the material hardens or softens with further deformation. The objective of this effort is to develop a consistent description of the dependence of dislocation mobility on the material crystal structure (e.g., BCC, FCC, or HCP), the applied stress and its orientation, the temperature and influence of alloying elements. Such task seems to be daunting at first sight. However, we will use guidance of theory, together with experimental measurements and computer simulations (Molecular Statics, Molecular Dynamics, and First Principles) to establish a semi-phenomenological database for dislocation mobility as a key input to DD simulations. In this first report, we focus on the dislocation mobility in tungsten single crystals.

The approach we will take here is that we will consider two regimes of dislocation motion. The first is at low values of stress and temperature, where dislocations can only move via kink pair nucleation and migration. This regime is characterized by the Peierls Stress (PS) at 0 K, and the thermal component of the Critical Resolved Shear Stress (CRSS) at any given temperature. The values of PS and CRSS are material dependent, and are very low for FCC metals, intermediate for HCP, and significant for BCC metals. At stress levels below the CRSS, dislocation motion is diffusive with a bias driven by the applied stress. If the bias is too high (i.e., high stress), the thermally activated process of kink pair nucleation and migration becomes irrelevant, and the dislocation momentum is reduced as a result of the scattering of elastic phonon waves off of the dislocation as it moves. This mechanism of damping, which was first introduced by Leibfried, becomes the dominant mechanism of motion at relatively high stress values and at high temperatures. As the dislocation velocity approaches the transverse speed of sound, it loses energy by emitting elastic waves, and thus the velocity is limited by the sound speed. In the following, we sketch out the basic theoretical ingredients that explain these mechanisms, and follow that with a semi-phenomenological description for DD simulations.

PROGRESS AND STATUS

Introduction

Peirels introduced the concept of whole-sale motion of a dislocation as a string above a sinusoidal barrier at absolute zero temperature. The dislocation line is assumed to be pushed rigidly over an atomic sinusoidal barrier. We discuss here the theoretical background behind the Peierls stress at absolute zero temperature. At finite temperatures, dislocation lines nucleate kinks and can move easier by kink nucleation and sideway motion.

Following Dorn and Rajnak [1], the energy per unit length of the dislocation can be approximates by a sinusoidal function of the form:

$$\Gamma(y) = \frac{\Gamma_c + \Gamma_0}{2} + \frac{\Gamma_c - \Gamma_0}{2}\left(\frac{\alpha}{2} + \cos\frac{2\pi y}{a} - \frac{\alpha}{4}\cos\frac{4\pi y}{a}\right) \tag{1}$$

where Γ_c and Γ_0 are the energies at the top and bottom of the Peierls hill, α is a factor that controls the shape of the potential, and a the lattice constant, as shown in Fig. 1. The three parameters, Γ_c, Γ_0, and α, can be readily obtained by fitting MS or First Principles data. Once

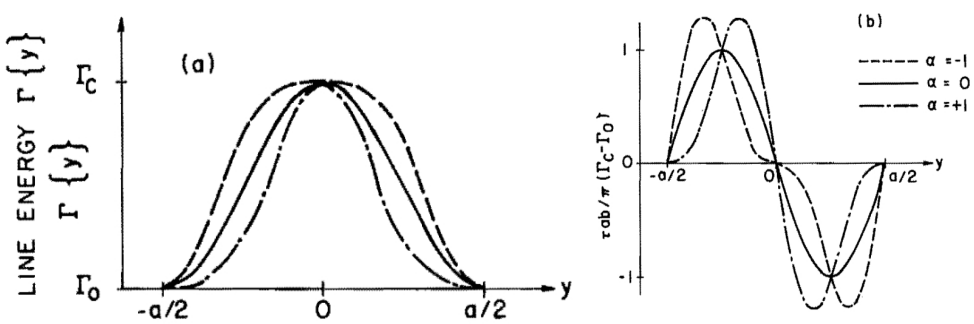

Figure 1. Illustration of Peierls Barrier (after Dorn & Rajnak).

obtained, and taking the derivative of Eq. 1, we obtain the PS as the maximum value of the energy derivative. Thus,

$$\tau_p b = \frac{\Gamma_c - \Gamma_0}{|\alpha| a}\frac{\pi}{16}\left(3 + \sqrt{1+8\alpha^2}\right)\sqrt{8\alpha^2 - 2 + 2\sqrt{1+8\alpha^2}} \tag{2}$$

In the special case of a sinusoidal energy profile ($\alpha = 0$), and taking the minimum energy $\Gamma_0 = 0$, we obtain a simple relationship between the Peierls stress and the Peierls energy barrier Γ_c:

$$\tau_p = \frac{\pi \Gamma_c}{\sqrt{2}ab} \tag{3}$$

There is some confusion in the literature as to the meaning of the Peierls Stress (PS), the flow stress (or Critical Resolved Shear Stress - CRSS), and how they depend on temperature and strain rate. For the purposes of facilitating DD computer simulations, we adhere to the strict definition of the Peierls Stress as *the stress required to move the dislocation rigidly across an atomic potential barrier at absolute zero*. As the temperature increases, fluctuations cannot be suppressed and dislocation motion will naturally move by the generation and motion of kink pairs. However, if the strain rate is very high (as in MD simulations, for example), the dislocation must generate higher and higher concentrations of kink pairs to keep up with the applied strain rate. Thus, for a given temperature and a high enough strain rate, there will be a stress at which the dislocation appears to move as a whole again (similar to the Peierls concept at absolute zero), and the applied stress will be balanced by phonon drag alone (no short range atomic barrier). This situation coincides with the thermal regime of plastic flow measured experimentally in single crystals. We will refer to this critical stress value as the Kink Saturation Stress (KSS), or $\tau_K(T)$. Finally, the CRSS (or flow stress), is *the stress at which dislocations move so as to keep up with an applied strain rate*. The CRSS is temperature and strain rate dependent, and has a thermal ($\tau^*(T)$), and an athermal, or friction (τ_F) component. At very high temperatures (above $\approx 0.7\,T_m$), the CRSS decreases as a result of vacancy diffusion.

Theory of Dislocation Motion

Kink-Pair Formation

Because in the first regime dislocation motion is governed by the motion of kinks, we consider the theoretical background of kink formation and migration under applied stress. We then determine the velocity of kinks and finally express the dislocation velocity in terms of the kink velocity. The kink formation energy is the difference in the dislocation line energy from its straight configuration at the bottom of the Peierls hill (Γ_0), as shown in Fig. 2, thus:

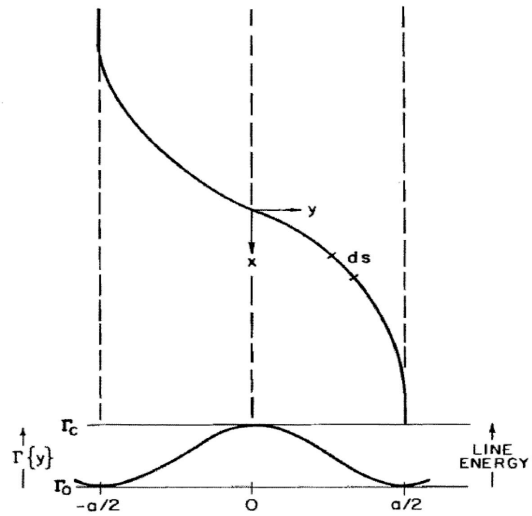

Fig. 4—A stable isolated kink under zero stress.

Figure 2. A stable isolated kink (after Dorn & Rajnak [1]).

$$U_k = \int_{-\infty}^{+\infty} \Gamma\{y\} ds - \Gamma_0 dx = \int_{-\infty}^{+\infty} f(y(x)) dx \tag{4}$$

This is a functional of the shape (y(x)), that can be minimized using $\delta U_k = 0$, which gives the Euler condition:

$$\frac{\partial f}{\partial y} - \frac{d}{dx}\frac{\partial f}{\partial y'} = 0 \tag{5}$$

The solution of Eq. 5 should result in uniquely determining the shape of the bent dislocation line with a kink on it, but ignores energy differences between the screw one edge components. The kink pair formation energy is given by:

$$U_k = \Gamma_0 \int_{-a/2}^{+a/2} \left(\sqrt{\left(\frac{\Gamma\{y\}}{\Gamma_0}\right) - 1}\right) dy \tag{6}$$

In the special case of $\alpha = 0$, this last equation can be integrated to give a closed form expression for the kink pair formation energy in a parametrized form:

$$U_k = \frac{\Gamma_0 a}{\pi}\left(\sqrt{2(R-1)} + (R+1)\tan^{-1}\sqrt{\frac{R-1}{2}}\right) \tag{7}$$

where $R = \Gamma_c / \Gamma_0$.

The energy required to nucleate a pair of kinks in the presence of an applied shear stress that is smaller than the Peirels stress ($\tau^* < \tau_p$) is given by the excess line energy from the straight configuration less the amount of work done by the shear stress in moving the kink pair across the Peierls barrier, thus:

$$\Delta H = \int_{-\infty}^{+\infty} \left(\Gamma\{y\} \sqrt{1 + (\frac{dy}{dx})^2} - \Gamma\{y_0\} - \tau^* b(y - y_0) \right) dx \tag{8}$$

Again, when we minimize the energy functional utilizing Euler's equation, a closed form expression for the line slope $\frac{dy}{dx}$ is obtained as:

$$\frac{dy}{dx} = \pm \sqrt{\left(\frac{\Gamma\{y\}}{\tau^* b(y - y_0) + \Gamma\{y_0\}} \right)^2 - 1} \tag{9}$$

Now, when Eq. 9 is substituted back into Eq. 8, the formation enthalpy of a kink pair is obtained as:

$$\Delta H_k^* = \int_{-\infty}^{+\infty} \left[\frac{(\Gamma\{y\})^2}{\tau^* b(y - y_0) + \Gamma\{y_0\}} - \Gamma\{y_0\} - \tau^* b(y - y_0) \right] dx \tag{10}$$

Dorn and Rajnak performed numerical evaluations of the integral, and the results are shown in Fig. 3.

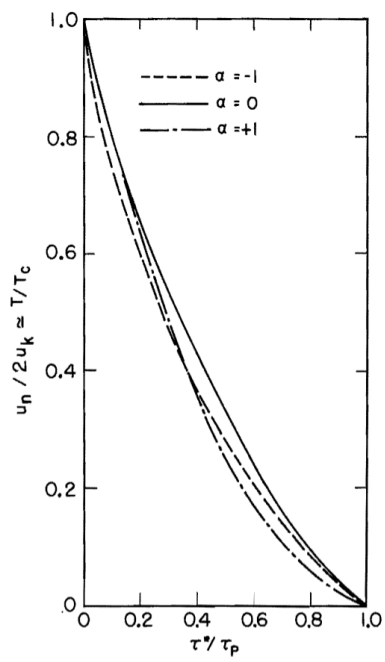

Figure 3. Kink Nucleation Enthalpy as a function of applied shear stress (after Dorn & Rajnak [1]).

The treatment presented above of Dorn and Rajnak assumes that the dislocation takes on a critical configuration to produce a kink pair that is not well-separated. Accurate line energy calculations of such critical configuration are difficult. If the critical configuration involves two well-separated kinks, separated a distance x apart on the dislocation line, the kink pair nucleation energy of this configuration will be:

$$\Delta H_k(x) = 2U_k - \frac{\mu b^2 h^2}{8\pi x} - \sigma b h x \tag{11}$$

This dependence of the formation enthalpy on x has a maximum at $x^* = (\frac{\mu b h}{8\pi\sigma})^{1/2}$, which, when substituted back into the previous equation yields:

$$\Delta H_k^* = 2U_k - \left(\frac{\mu\sigma b^3 h^3}{2\pi}\right)^{1/2} \tag{12}$$

If we approximate both b^3 and h^3 as Ω, the atomic volume, the previous equation takes a simple interpretation, as follows. If we define a mean stress $\sigma_m = \sqrt{\sigma\mu}$, then the work done by this stress on an atomic volume is $W_\sigma = \sigma_m \Omega$, and this mean stress decreases the kink pair nucleation energy by this amount of work, i.e.

$$\Delta H_k^* \approx 2U_k - \sigma_m \Omega = 2U_k - \left(\frac{\mu b^3 h^3}{2\pi}\right)^{1/2} \sqrt{\sigma} \tag{13}$$

The result of this last Eq. 13 is in qualitative agreement with the previous numerical estimation, given by Eq. 10. Both are indicative of a cut-off stress above which kink pair nucleation is thermal (The Peierls stress). However, Dorn and Rajnak's treatment expressed by Eq. 10 is more transparent, because of the explicit dependence on the CRSS (Peirels stress), which is itself a function of temperature.

If we take the activation energy for kink migration as E_k^m, then the jump frequency of kinks is:

$$\omega \approx \nu \exp(-\frac{E_k^m}{kT}) \tag{14}$$

Although ν is the attempt frequency of a kink jump (which depends on how widely separated a kink pair is), it can be roughly taken as the Debye frequency ν_D. The Debye frequency is an indication of how stiff the elastic medium is in propagating sound waves, and is interpreted as the highest frequency of phonons in the solid. This is associated with the shortest phonon wave, on the order of several ($\approx 2a$) lattice constants. It is obtained from the Debye temperature as: $kT_D = h\nu_D$, where T_D is the Debye temperature, and h is Planck's constant. The diffusion coefficient of kinks is simply $D_k = \beta a^2 \omega$, where β is a numerical factor. Under applied force, the diffusion of kinks becomes biased by the force and the velocity is described by the mobility of a kink in an applied force field, namely:

$$v_k = \frac{D_k}{kT} F = \frac{D_k}{kT} \sigma bh \approx \nu_D b^2 \exp(-\frac{E_k^m}{kT}) \frac{\sigma bh}{kT} = \exp(-\frac{E_k^m}{kT}) \frac{\sigma \nu_D b^4}{kT} \tag{15}$$

Here, we took $h \approx b$. Since the transverse sound speed is $C_t \approx \nu_D b$, and since there is evidence that kinks move even at temperatures close to absolute zero, then we will also take the limit that $E_k^m << kT$, making the exponential term to be nearly unity. The kink velocity is then:

$$v_k \approx C_t (\frac{\sigma \Omega}{kT}) \tag{16}$$

where C_t is the transverse sound speed. The same result of Eq. 16 can also be obtained from Leibfried's theory of momentum transfer by elastic wave scattering, which we will outline later. A simpler way of remembering this result is to scale the stress by Ω/kT and the velocity by C_t. Thus, if we define scaled stress and velocity, respectively, as: $\tilde{v}_k = v_k/C_t$, and $\tilde{\sigma} = \sigma\Omega/kT$, we have:

$$\tilde{v}_k = \tilde{\sigma} \tag{17}$$

Dislocation Velocity

If one takes the concentration of positive and negative kinks to be equal, then $C_k = \frac{2}{a}\exp(-\frac{\Delta_k^*}{kT})$. Let's assume that a kink has moved a distance X along the dislocation line till it recombines with another average kink, making the dislocation move forward a distance h at a velocity v. The area swept by the kink lateral motion must be the same as that swept by the motion of the dislocation line, $vX = v_k h$. This simple argument gives the dislocation velocity as a function of the kink velocity;

$$v = \frac{h}{X} v_k \tag{18}$$

The distance X is the inverse of the kink concentration on the dislocation line, C_k. Therefore, we can now develop a simple equation for the velocity of a dislocation:

$$v = \frac{2\sigma b h^2}{akT} D_k \exp(-\frac{\Delta H_k^*}{kT}) \tag{19}$$

Substituting for the kink diffusivity $D_k \approx \nu_D a^2$, and ignoring geometric differences between a, h, and b, we obtain the following approximate equation for the dislocation velocity:

$$v = \frac{2\sigma\Omega}{kT} \nu_D a \exp(-\frac{\Delta H_k^*}{kT}) \tag{20}$$

Because we are looking for a semi-phenomenological description, and because of the numerocal uncertainties in the forgoing theoretical treatments, we will re-write Eq. 20 as:

$$v = \zeta(\frac{\sigma\Omega}{kT}) \exp(-\frac{\Delta H_k^*}{kT})(\nu_D a) \tag{21}$$

where ζ is a numerical factor. The last equation (Eq. 21) is written in this form to emphasize the origin of the dislocation velocity being determined by the success of kink jumps at the Debye frequency over an atomic distance, biased forward by the ratio of the work done on an atomic volume to that in thermal vibrations. As we did earlier for the kink velocity, we can also use

scaled variables for the dislocation velocity if we remember that the product of the Debye frequency and the lattice constant is approximately the transverse sound speed, C_t. Thus, in scaled variable form, the scaled dislocation velocity is:

$$\tilde{v} = \zeta\tilde{\sigma}\exp(-\frac{\Delta H_k^*}{kT}) \tag{22}$$

<u>The nucleation theory approach</u>

To complete this theoretical description and put it in perspective, we can also develop the same equation for the dislocation velocity (Eq. 22) from considerations of classical nucleation theory of kinks on the dislocation line. Here we follow the treatment given by Hirth and Lothe.

According to classical nucleation theory, the constrained equilibrium concentration of kink pairs (without mutual interaction) is given by:

$$C_p = C_k^+ C_k^- = \frac{1}{a^2}\exp(-\frac{\Delta H_k}{kT}) \tag{23}$$

The main result of classical nucleation theory is that the nucleation rate of kinks, J_k is only determined by the kink concentration at the saddle point and the critical size of a kink pair, x_{crit}. This critical size is the size that overcomes thermal fluctuations, i.e., given by:

$$\sigma b h x_{crit} \approx kT \tag{24}$$

The kink nucleation rate is:

$$J_k \approx \frac{2D_k C_p(x^*)}{2x_{crit}} = \frac{\sigma b h}{a^2 kT} D_k \exp(-\frac{\Delta H_k^*}{kT}) \tag{25}$$

If the average distance travelled on the dislocation line before kinks are annihilated is X, the dislocation velocity is the average distance a dislocation line of unit length advances per unit time. Such average distance is simply the area swept by a kink pair times the rate at which kink pairs are created per unit time, thus:

$$v = hXJ_k \tag{26}$$

Howver, the distance X is dependent on the average lifetime of a kink pair $X = 2v_k\tau$, and $\tau = 2/J_k X$, which gives:

$$X = 2(\frac{v_k}{J_k})^{1/2} \tag{27}$$

Which, when inserted into Eq. 26, gives:

$$v = 2h(J_k v_k)^{1/2} = \zeta(\frac{\sigma\Omega}{kT})\exp(-\frac{\Delta H_k^*}{kT})(\nu_D a) \tag{28}$$

which is now identical to Eq. 22.

Dislocation Motion Limited by Phonon Interactions

At high stress, the velocity is controlled by dislocation interaction with elastic waves and damping results from momentum loss. We will first consider the thermally-activated regime, where kinks are created on dislocation lines, and the dislocation as a whole moves when these kinks glide and annihilate along the dislocation line itself. At high stresses and temperatures, the dislocation is dragged in a phonon gas, which results in imparting damping properties on dislocation motion by a number of mechanisms.

Leibfried's Phonon Scattering Theory

The theory of Leibfried [2] mimics the idea of momentum loss of electromagnetic waves upon scattering from objects of a finite cross-section. We briefly summarize the idea her. Consider a plane shear wave: $u_z = A\cos(k \cdot r - \omega t)$. The momentum density of the wave is $g = \frac{1}{2}\omega A^2 k$. If we assume that the dislocation has a scattering cross-sectional area of approximately D per unit length, and an elastic wave of energy density $w = \frac{1}{2}\rho_0 \bar{\dot{u}}^2$. For a wave train of length $L = C_t t$, the transmitted wave train contains less energy after scattering by the amount DLw, and hence less momentum by the amount $DLwt$, where t is the scattering time. Per unit length, the momentum loss in scattering the elastic wave is:

$$\Delta M/L = Dtw \tag{29}$$

and the force imparted to the dislocation during this impulse is simply $F/L = \Delta M/Lt = Dw$. Leibfried found that balancing this scattering radiation force against damping due to thermal vibrations requires that the scattering cross-section D be on the order of $b/10$, and that the elastic energy per unit time ($wC_t D^2$) must be lost to the energy contained in the volume swept by dislocation motion per unit time ($w_T v D^2$), where $w_T = 3kT/\Omega$ is the average thermal energy density. Thus:

$$wC_t = w_T v \tag{30}$$

Therefore, an estimate for the force per unit length of the dislocation under this momentum balance assumption is:

$$F/L = \sigma b = \frac{w_T b}{10}\frac{v}{C_t} \tag{31}$$

or,

$$\tilde{v} = 10\sigma/w_T = 10\sigma\Omega/3kT = \frac{10}{3}\tilde{\sigma} \tag{32}$$

Apart from the numerical factor of $\frac{10}{3}$, this form of Leibfried's equation is essential the same as the kink velocity equation we showed earlier (Eq. 17).

Phonon Gas Viscosity

In this approach, damping of elastic waves in the solid is considered to result from an effective phonon viscosity. Mason [3] extended this idea to model the damping of a moving dislocation, where the dislocation is assumed to be dragged in a phonon gas. Thus, the classical kinetic theory of gases and the Debye model of the specific heat can be used to construct an equation for dislocation viscosity.

The key results of the kinetic theory of gases are as follows:

$$\lambda = \frac{3K}{C_v \overline{C}_s} \tag{33}$$

$$\eta = \frac{NM\lambda}{3} \tag{34}$$

where λ is the phonon mean free path, K the thermal conductivity, C_v the specific heat at constant volume, $\overline{C}_s$ is an average sound speed $\overline{C}_s^3 = C_t^3(3/(2 + C_T^3/C_L^3))$, η is the viscosity, N the number of phonons and M their momentum; $M = \hbar\omega/\overline{C}_s$. Using these results of kinetic theory, the dislocation viscosity is found as:

$$\eta = \frac{N\hbar\omega\lambda}{3\overline{C}_s} = \frac{E_0\lambda}{3\overline{C}_s} = \frac{kT\lambda}{3\Omega\overline{C}_s} \tag{35}$$

where $E_0 = kT/\Omega$ is the thermal energy in the phonon gas per unit volume. Since the force on the dragged dislocation, $F = \sigma b$, must be balanced by viscous drag ηv, where v is the dislocation velocity, then we have:

$$v = \frac{\sigma b}{\eta} = \frac{3\sigma b\Omega\overline{C}_s}{kT\lambda} \tag{36}$$

This last equation can again be cast in scaled variables as:

$$\tilde{v} = \frac{3}{\tilde{\lambda}}\tilde{\sigma} \tag{37}$$

where $\tilde{\lambda} = \lambda/b$. The remarkable resemblance of Eq. 37, which is purely based on the kinetic theory of gases, and Leibfried's formula (Eq. 32), which he developed from scattering theory, indicates that the phonon mean free path in Leibfried's theory must be on the order of one lattice constant for the two approaches to be equivalent. Although Leibfried's formula is used in some estimates of dislocation mobility in the literature, Eq. 37 that we developed here based on

Mason's work may be more useful. For example, size effects do not show up in Leibfried's formula, but they can affect the interpretation of MD simulation data, where the mean phonon free path length is dependent on the simulation size. What remains now is a method to determine $\tilde{\lambda}$ from thermodynamic materials data for large crystals, or from MD data for small systems. Following the kinetic theory results above, the phonon mean free path length is determined by knowing the thermal conductivity, the specific heat at constant volume and the average sound speed. However, since in reality we have tow interacting gases; the phonon and electron gases, we would need to just consider the contributions of the phonon gas to the conductivity and specific heat. In metals, the thermal conductivity is dominated by electrons, while the specific heat is dominated by the phonons. Mason expressed the specific heat of electrons as $C_{ve} = \beta T$, and showed that when the ratio of the electron to phonon thermal conductivity are used, the phonon mean free path length from thermodynamic data can be found as:

$$\lambda = \frac{3\overline{C}_s K}{bC_{ve}V_F^2} = \frac{3\overline{C}_s K}{b\beta T V_F^2} \tag{38}$$

where V_F is the electron Fermi velocity:

$$V_F = \frac{\hbar(3\pi^2)^{1/3}}{\Omega^{1/3} m} \approx \frac{\hbar(3\pi^2)^{1/3}}{bm} \tag{39}$$

and m is the electron mass. We note that the specific heats are per unit volume. When this is substituted back into the previous equation, we get:

$$\lambda \approx \frac{\overline{C}_s K b^2 m^2}{b\hbar^2 \beta T} \tag{40}$$

In scaled units;

$$\tilde{\lambda} \approx \frac{\overline{C}_s K m^2}{\hbar^2 \beta T} \tag{41}$$

This finally mans that we need to use the thermal conductivity, the average sound speed, and the β constant that describes the electronic specific heat in order to determine $\overline{\lambda}$.

A phenomenological model of dislocation velocity

Our next goal is to utilize the theoretical forms and understanding to represent the dislocation mobility data in DD simulations. We would thus be using a phenomenological approach, where the velocity equations are fitted either from experimental data or from MD simulations, guided by the theoretical understanding presented in the previous section. A similar law was determined by numerical integration by Dorn and Rajnak for a different Peierls potential. For generality we shall use the following fit [4]:

$$\Delta H^* = \Delta H_0 \left[1 - \left(\frac{\sigma}{\tau_p} \right)^p \right]^q \tag{42}$$

We now wish to find the *stress necessary to sustain a given plastic strain rate for a given temperature by the double kink mechanism*. To this end, we consider the plastic strain rate in the thermally-activated regime in the form:

$$\dot{\gamma} = \dot{\gamma}_0 \exp\left(-\frac{\Delta G^*}{kT} \right) = \dot{\gamma}_0 \exp\left(-\frac{\Delta H^* - T\Delta S^*}{kT} \right) \tag{43}$$

where ΔS^* is the activation entropy. Now plug (42) into (43) and solve for σ. This gives:

$$\sigma(T) = \tau_p \left[1 - \left(\frac{T}{T_a} \right)^{\frac{1}{q}} \right]^{\frac{1}{p}} \tag{44}$$

where the "athermal" temperature, T_a is given by:

$$T_a = \frac{\Delta H_0}{\Delta S^* + k \ln \frac{\dot{\gamma}_0}{\dot{\gamma}}} \tag{45}$$

We now note that when $\dot{\gamma}$ is the maximum plastic strain rate allowed by the double kink mechanism ($= \dot{\gamma}_0$), we obtain $T_a = \frac{\Delta H_0}{\Delta S^*}$. Since ΔS^* s related to changes in vibrational frequencies of the crystal during the kink formation process, then T_a must be a function of the Debye temperature. Assuming a linear dependence, we consider $T_0 = mT_D$, where T_D is the Debye temperature and m is approximately 2. However, if we consider entropic effects (Seeger, 1955), we would have to modify the dependence of T_a on strain rate.

The experimental data and MD simulations for dislocation velocity show a consistent behavior that can be modeled in a universal phenomenological law. We will utilize both MD simulations and experimental data on single crystals to determine the dynamic PS, as a function of temperature. Since T_a scales inversely with the logarithm of the strain rate (See Eq. 46), then we may write it phenomenologically as:

$$T_a = \frac{mT_D}{\left(1 + \ln \frac{\dot{\gamma}^{sat}}{\dot{\gamma}} \right)} \tag{46}$$

where T_D is the Debye temperature, and $\dot{\gamma}^{sat}$ is the "kink saturation" strain rate, which can be set at $10^7\ s^{-1}$. The MD results (say at $\dot{\gamma} = 10^7 s^{-1}$) can be used with other experimental data in the scaling relationship. Let's now account for thermal activation effects on the stress by introducing a second scaled stress given by:

$$\tilde{\tilde{\sigma}} = \tilde{\sigma} \exp(-\frac{\Delta H_k^*}{kT}) \tag{47}$$

To reproduce the two velocity regimes, and to account for differences in the mechanisms of kink motion between edge and screw components, we will describe the activation energy for kink nucleation, as follows:

$$\Delta H_k^*(\tau) = \left[U(0) - U(\tau_P(T))\right] \Delta H_0(T) \left[1 - \left(\frac{\sigma}{\tau_p(T)}\right)^p\right]^q \tag{48}$$

This last equation is quite universal, because it accounts for transitions between the kink-dominated and phonon-drag dominated velocity regimes through the introduction of the unit step functions: $U(0)$ and $U(\tau_P(T))$. It also accounts for a gradual velocity mechanism transition between screw and edge components through the $\cos$ angle between the tangent and Burgers vectors of the dislocation, b and t, respectively. Once this universal kink nucleation energy is calculated, and to account for acoustic radiation losses that limit dislocation velocities to the average sound wave speed at high stress, the following universal law is proposed:

$$\tilde{v} = 1 - \exp(-\frac{3\tilde{\tilde{\sigma}}}{\tilde{\lambda}}) \tag{49}$$

It is noted that the fitting parameters that lead to Eq. 49 are here interpreted as a function of the dislocation line orientation (screw or edge), and may also be distinguished for different families of slip systems. The remarkable simplicity of Eq. 49 and its ability to capture the stress and temperature dependence of both screw and edge dislocations in BCC, FCC, and HCP metals makes it a good candidate for inclusion in DD simulation computer programs.

The calculation algorithm for the dislocation velocity would now be simple, and as follows. For a given stress, temperature, crystal structure, slip plane, dislocation orientation, and material, we first calculate the scaled stress, $\tilde{\sigma}$. Next, we find the Peierls and phonon-drag stress (which can be very low for FCC metals). Knowing the kink nucleation energy at absolute zero, ΔH_1, we can calculate ΔH_k^*, and hence the scaled stress $\tilde{\tilde{\sigma}}$. Then, we determine the scaled phonon m.f.p $\tilde{\lambda}$ from Eq. 41. Finally, we apply the universal velocity equation, given by Eq. 49.

RESULTS

The CRSS [4] for tungsten has been determined by Dorn and Rajnak [1], Lassner [5], and Brunner [6]. The results are obtained at different strain rates, and refelct some starin rate

effects, as shown in Figure (4). In addition, we also determined the CRSS from our MD simulations of pure tungsten by an extrapolation procedure of the dynamics velocity data. The MD results are also consistent with a strain rate shift of the CRSS, as can be seen in Figure (4).

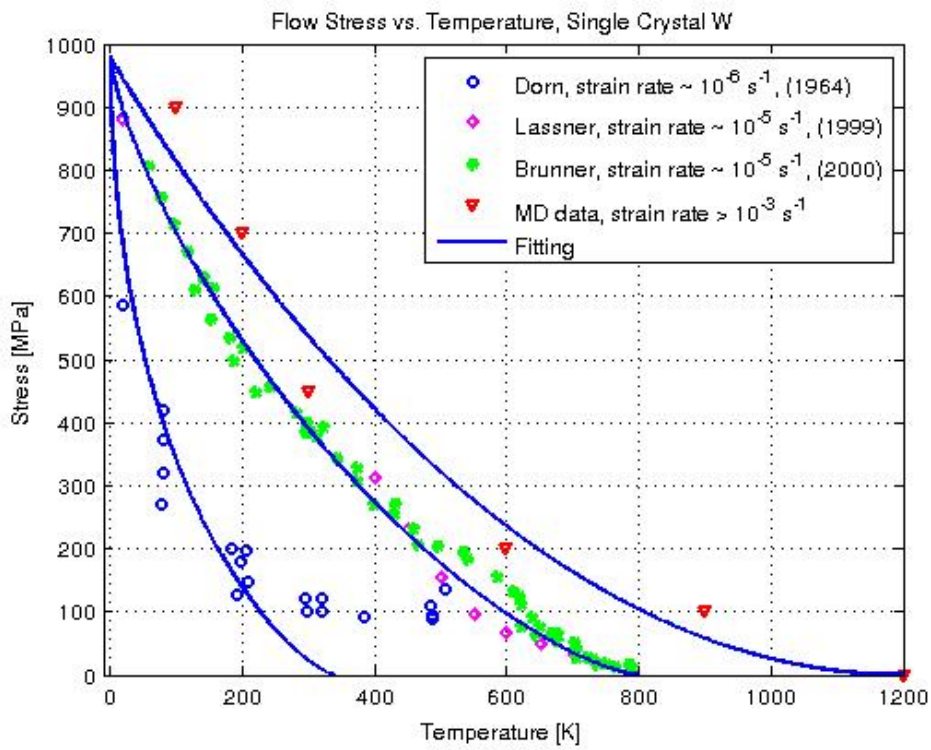

Figure 4. Plot showing flow stress data taken from Dorn 1964 and Lassner 1999, the blue circles correspond to the raw data taken from fig.13 of Dorn 1964, while the magenta squares correspond to data taken from Lassner 1999 book. Red triangles correspond to MD data approaching high strain rate regime. The athermal temperature is defined as that at which the fitted curves intersect the x-axis, being $340K$ and $800K$ for Dorn and Lassner respectively. In addition, the fitting parameters p and q are $p = 0.51, \quad q = 1.26$ for Dorn, and $p = 1, \quad q = 1.69$ for Lassner data.

The data obtained from experimental sources, and those from MD simulations were fitted to Equations (44) for the CRSS, with Equation (46) for the characteristric temperature, T_a. This procedure can produce a universal CRSS versus the scaled temperature T/T_a, as shown in Figure (5). Except for a few data points, the univbersal fit is consistent with the proposed model.

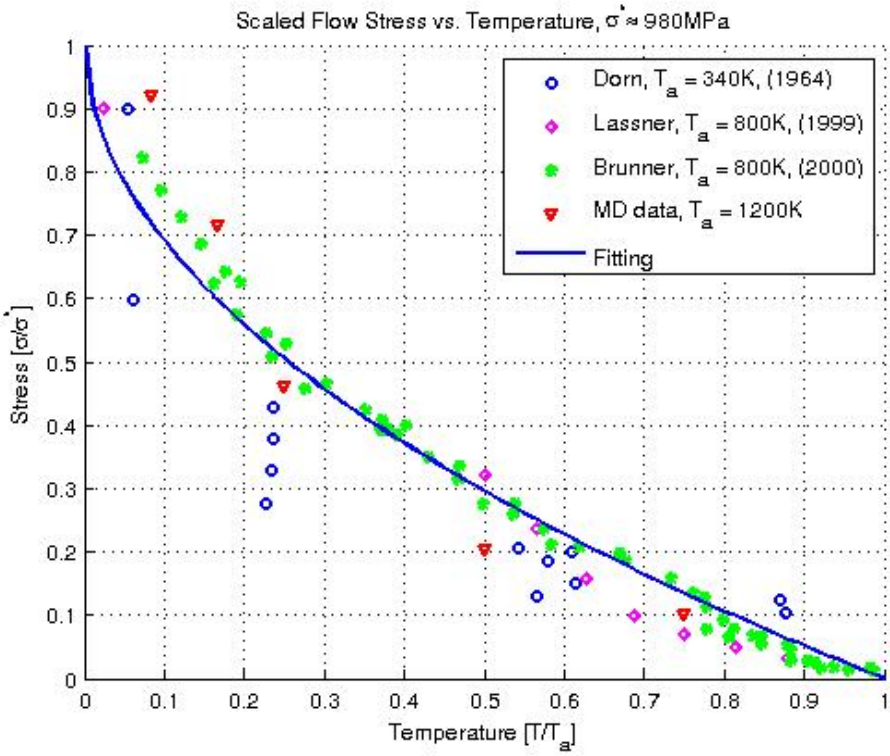

Figure 5. Normalized flow stress vs. Temperature, data in figure 4 is scaled by their respective athermal temperature and Peierl's stress (approx 980 MPa). As can be seen, all the data collapses into one master curve, which can be fitted with the aid of equation 44. The fitting parameters are q = 2 and p = 1.

Figure (6) shows the results of the model for the screw dislocation velocity in tungsten at any applied stress and temperature. The results indicate that the kink nucleation and motion regime is very limited to low stress and temperature combinations. That may be one of the reasons that MD simulations can best give information on the phonon drag mechanism rather that the kink pair nucleation mechanism.

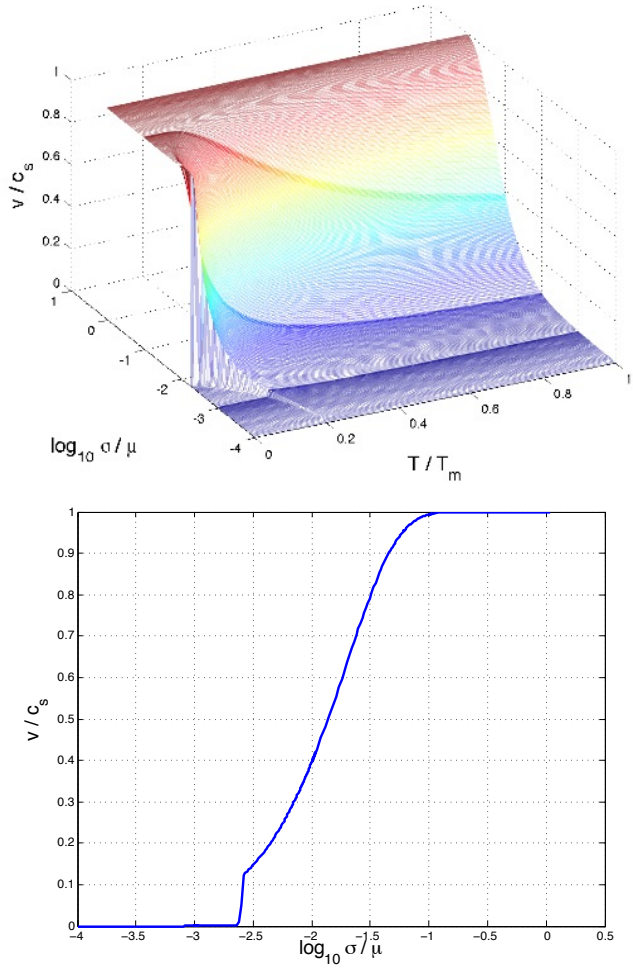

Figure 6. Dislocation velocity (normalized by $c_s = 2890\,m/s$) of screw dislocations in W. a) Velocity as a function of applied stress and temperature. b) Dislocation velocity at 300K. Threes regimes are distinguishable: the kink-pair regime, the phonon drag regime, and the regime characterized by energy radiation.

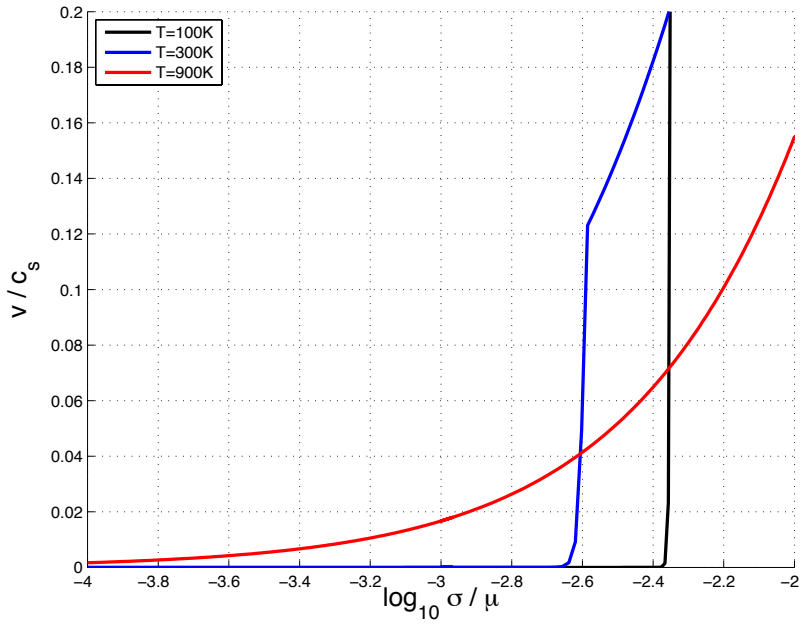

Figure 7. Dislocation velocity in the low stress range, for three different temperatures. At T=100K, dislocations move by the kink mechanism only. At T=300K, the transition between the kink regime and the phonon regime is visible. At T=900K, dislocation motion is by phonon drag only.

Figure (7) shows the dislocation velocity as a function of applied stress for three different temperatures. In the low temperature regime, dislocations clearly move by the generation and motion of kink pairs. At 300 K, the transition between kink dominated motion and phonon drag is evident. At high temperature, dislocation motion is entirely dominated by phonon drag.

REFERENCES

[1] John Dorn and Stanley Rajnak, "Nucleation of Kink Pairs and the Peierls' Mechanism of Plastic Deformation," Transactions of the Metallurigical Society of AIME, 320, 1052-1064, 1964.

[2] Gunther Leibfried, "Uber den Einfluss thermisch angeregter schallwellen auf die plastische deformation, -On the influence of thermally excited sound waves on the plastic deformation," *Zeitschrift fur Physik*, **127**, 344-356, 1950.

[3] Warren Mason, "Phonon viscosity and its effect on acoustic wave attenuation and dislocation motion," *The Journal of the Acoustical Society of America*, **32(4)**, 458-472, 1960.

[4] Kocks, U., Argon, A., & Ashby, M. (1975). Thermodynamics and Kinetics of Slip. Progress in Materials Science, 19, 1–281.

[5] Erik Lassner and Wolf-Dieter Schubert, "Tungsten, Properties, Chemistry, Technology of the Element, Alloys, and Chemical Compounds", Kluwer Academic / Plenum Publishers 1999.

[6] Brunner, Dieter, "Comparison of flow-stress measurements on high-purity tungsten single crystals with the kink-pair theory", Materials Transactions, JIM(Japan) 41 1 152-160.