Supersonic Dislocation Kinetics from an Augmented Peierls Model

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The controversial issue of whether dislocations can travel faster than shear or longitudinal waves is investigated. The Peierls model, modified to account for drag and gradient effects, furnishes a kinetic relation between the applied shear stress and speed of uniformly moving dislocations. This relation predicts intersonic and supersonic speeds at high enough stress, but also regimes of unstable motion, in agreement with recent atomistic simulations.

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The propagation of dislocations, twins, and cracks in solids at speeds higher than that of shear waves has long been considered unlikely. This belief is based on predictions of linear elastic models [1] that ignore nonlinearity, nonlocality, and lattice discreteness, factors that play a crucial role in defect structure and dynamics. Indeed, recent experiments detected intersonic crack speeds [2] (between the shear wave speed c_S and the longitudinal wave speed c_L), while atomistic simulations predicted intersonic and supersonic dislocations (faster than c_L) [3,4]. Intersonic twins have also been observed [5], simulated [6], and analyzed [7].

An important question raised by the pioneering studies of dislocation dynamics [8,9] is whether the speed of a moving dislocation can be determined as a function of the applied stress. We show that the Peierls dislocation model, augmented to include drag and gradient effects in a simple way, determines an explicit kinetic relation between the dislocation speed and the externally applied shear stress. In the subsonic speed range, this relation exhibits a low-speed, drag-dominated regime and a high-speed relativistic regime in qualitative agreement with experimental observations. Intersonic motion is predicted to occur above a critical applied stress, but is unstable below a critical speed. Supersonic propagation takes place above a higher critical stress level. These results explain recent observations of atomistic simulations [4] through a physically simple, analytically tractable continuum-mechanical model. The prediction of dislocation kinetics is relevant to the dynamics of twinning, martensitic transitions, and viscoplastic behavior of solids.

The Peierls model [10] is a continuum analog of a dislocated crystal: two linear elastic isotropic half-spaces are joined along a slip plane with a nonlinear *interface law* $\sigma = f(u)$, expressing shear traction σ as a periodic function of slip displacement u. When applied to uniformly gliding *edge* dislocations, it yields Weertman's equation [9] for the slip displacement $u(x - vt)$:

$$\frac{\mu}{\pi} A(v) \int_{-\infty}^{\infty} \frac{u'(z)}{z - x}\, dz + \mu B(v) u'(x) + \sigma_{\mathrm{appl}} = f(u(x)) \,. \tag{1}$$

Here $v \geq 0$ is the constant glide speed; we write x in place of the moving coordinate $x - vt$; primes indicate differentiation; $f(u) = \Phi'(u)$ is the derivative of a periodic *interface potential* $\Phi(u)$ with period the Burgers vector b; μ is the shear modulus; σ_{appl} is the externally applied constant shear stress parallel to the slip plane; letting $\beta_i = |1 - (v/c_i)^2|^{1/2}$, $c_1 = c_L$, $c_2 = c_S$, $c_3 = \sqrt{2}\, c_S$, the functions $A(v)$ and $B(v)$ are given by

$$A(v) = \begin{cases} 2(c_S/v)^2(\beta_1 - \beta_3^4/\beta_2), & 0 < v < c_S\,, \\ 2(c_S/v)^2\beta_1, & c_S \leq v < c_L\,, \\ 0, & c_L \leq v < \infty\,, \end{cases}$$

$$B(v) = \begin{cases} 0, & 0 \leq v \leq c_S\,, \\ 2(c_S/v)^2\beta_3^4/\beta_2, & c_S < v < c_L\,, \\ 2(c_S/v)^2(\beta_1 + \beta_3^4/\beta_2), & c_L \leq v < \infty\,. \end{cases} \tag{2}$$

They arise in the solution of the steady elastodynamic problem in the half-spaces; $A(v)$ is a relativistic contraction factor, complicated by the presence of two wave speeds, and vanishes above c_L; $B(v)$ is the intensity of shear and longitudinal shock waves emitted by the dislocation core when v is above c_S and c_L, respectively, and vanishes below c_S. Solutions $u(x)$ of (1) corresponding to moving dislocations have limits

$$u(\infty) = u_0, \qquad u(-\infty) = b + u_0, \qquad u'(\pm\infty) = 0, \tag{3}$$

$$\text{where} \quad u_0 = \text{const}, \qquad f(u_0) = \sigma_{\mathrm{appl}}\,. \tag{4}$$

Necessary for stability of solutions is that the states $u = u_0$ far ahead of the dislocation and $u = b + u_0$ far behind it are statically stable, namely, $f'(u_0) \geq 0$ [11].

The search for combinations of σ_{appl} and v for which such solutions exist produces physically unappealing results, as we show next. The *energy dissipation rate* D for the system is the rate of external work done by σ_{appl} minus the rate of change of the total elastic, interfacial, and kinetic energy. A standard calculation shows that

$$D = Fv, \qquad F = \sigma_{\mathrm{appl}} b - \mu B(v) \int_{-\infty}^{\infty} [u'(x)]^2\, dx\,. \tag{5}$$

Here F is the *driving force* acting on the dislocation [12]. For subsonic motion ($v < c_S$) $B(v) = 0$ and F reduces to the Peach-Koehler force $\sigma_{\rm appl} b$. On the other hand, multiplying (1) by u' and integrating gives [13]

$$\sigma_{\rm appl} b = \mu B(v) \int_{-\infty}^{\infty} [u'(x)]^2 \, dx \,, \tag{6}$$

so that F and the dissipation rate D necessarily vanish for all solutions of (1). This reflects the conservative nature of the Peierls model: external work becomes elastodynamic energy of radiated shock waves. Since $B(v) = 0$ for $v < c_S$, Eq. (6) implies that subsonic motion would occur *at zero applied stress and at any speed* below the Rayleigh speed $c_R \approx 0.93 c_S$ [the subsonic surface-wave speed, such that $A(c_R) = 0$] [8]. The Peierls model lacks a drag mechanism, which would provide the resistance overcome by $\sigma_{\rm appl}$ to maintain motion when shock waves are absent. It implies that dislocations would move at intersonic speeds for arbitrarily small $\sigma_{\rm appl}$ [9]. It fails to predict a reasonable kinetic relation (between $\sigma_{\rm appl}$ and v) that should be monotone increasing for low subsonic speeds as expected from experiments [14]. The model does predict intersonic motion, but also that $\sigma_{\rm appl} = 0$ when $v = \sqrt{2}\, c_S$, the special intersonic speed at which no shock waves are emitted [$B(\sqrt{2}\, c_S) = 0$] [9]. It does not allow for supersonic motion, recently encountered in atomistic simulations [4]. We address these issues by proposing various extensions to the model.

Model 1.—We modify the interface law by adding a rate-dependent term $\bar{\alpha} \dot{u}$ to $f(u)$; $\alpha = \bar{\alpha} c_S/\mu > 0$ is a nondimensional viscosity parameter. Since $\dot{u} = -v u'$, this term is mainly active at the core; it is intended to account for phonon and electron drag [1] in a simple phenomenological way. The interface law now reads $\sigma = f(u) + \bar{\alpha} \dot{u}$. This replaces $B(v)$ in (1) and (6) by

$$B_\alpha(v) = B(v) + \alpha v/c_S \,. \tag{7}$$

The driving force in (5) becomes $F = \bar{\alpha} v \int_{-\infty}^{\infty} u'^2 \, dx$, yielding a positive dissipation rate $D = F v$. We make the usual choice

$$f(u) = \sigma_{\rm th} \sin(2\pi u/b) \,; \tag{8}$$

$\sigma_{\rm th} = \max f(u)$ is known as the *theoretical shear strength* [1]. A solution of the resulting version of (1) is

$$u(x) = u_0 + (b/\pi)[\pi/2 - \tan^{-1}(x/Dd)], \tag{9}$$

where $d = \mu b/2\pi\sigma_{\rm th}$, u_0 satisfies (4), while the core-size factor D and stress $\sigma_{\rm appl}$ are determined as functions of v:

$$D(v) = [A^2(v) + B_\alpha^2(v)]^{1/2}, \tag{10}$$

$$\sigma_{\rm appl}(v) = \sigma_{\rm th} B_\alpha(v)/D(v) \,, \tag{11}$$

with A, B, and B_α given by (2) and (7). When $v = 0$, $\sigma_{\rm appl} = 0$ and (9) reduces to the static Peierls solution [8] with $D(0) = 1/2(1 - \nu)$, where ν is Poisson's ratio. The *kinetic relation* between $\sigma_{\rm appl}$ and v is supplied by (11); it is equivalent to the relation $F(v) = b \sigma_{\rm th} \alpha v / D(v) c_S$ between the driving force in (5) and the speed.

In the *subsonic range* $0 \le v < c_S$, $\sigma_{\rm appl}(v)$ is monotone increasing for $0 < v < c_R$; see Fig. 1(a). It exhibits a low-speed drag regime; $\sigma_{\rm appl}(v) \approx \eta v/c_S$ for $v \ll c_S$, with drag coefficient $\eta = 2(1 - \nu)\alpha\sigma_{\rm th}$. As $v \to c_R$, $\sigma_{\rm appl}(v)$ increases steeply to the theoretical shear strength $\sigma_{\rm th}$ due to relativistic effects [$A(v) \to 0$ as $v \to c_R$]. These features of $\sigma_{\rm appl}(v)$ are consistent with experiments [14]. For $c_R < v < c_S$, $\sigma_{\rm appl}(v)$ has negative slope. Also u_0 is unstable, since one shows that $f'(u_0) < 0$. Hence, motion in the range $c_R < v < c_L$ is unstable.

In the *intersonic range* $c_S < v < c_L$ [Fig. 1(b)], $\sigma_{\rm appl}(v)$ decreases from $\sigma_{\rm appl}(c_S+) = \sigma_{\rm th}$ to a minimum at a speed v_*, then increases again to $\sigma_{\rm appl}(c_L) = \sigma_{\rm th}$. This is due to the behavior of the shock wave intensity $B(v)$, which has a minimum, and vanishes, at $v = \sqrt{2}\, c_S$. For $c_S < v < v_*$ motion is unstable [15]. Stable intersonic motion occurs for $\sigma_{\rm appl}$ above the critical value $\sigma_{\rm trans} = \sigma_{\rm appl}(v_*) > 0$ at speeds $v_* < v < c_L$. The critical speed v_* is always below $\sqrt{2}\, c_S$, but approaches it, while $\sigma_{\rm trans} \to 0$, as the viscosity $\alpha \to 0$. For $\alpha \ll 1$, $v_* \approx \sqrt{2}\, c_S$, while $\sigma_{\rm trans} \approx 2\alpha\sigma_{\rm th}$. Thus $\sigma_{\rm trans} > 0$ due to drag effects; wave effects increase $\sigma_{\rm appl}$ further for $v > v_*$. No supersonic motion is possible in this model at stresses below $\sigma_{\rm th}$ with u_0 stable [16].

Model 2.—A nonlocal dependence of the interface potential on the slip displacement was considered in [17] in

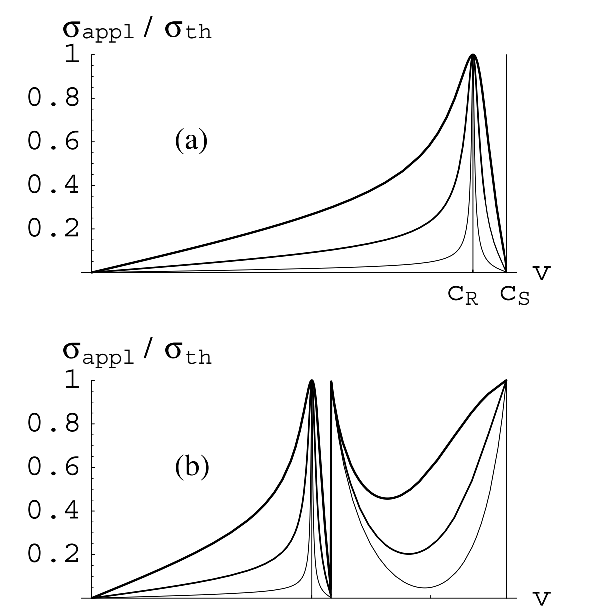

FIG. 1. The kinetic relation of model 1, $\sigma_{\rm appl}/\sigma_{\rm th}$ versus v from Eq. (11), for different values of viscosity $\alpha = 0.02$, 0.1, 0.3, shown thicker for higher α. (a) Subsonic range $0 \le v \le c_S$. (b) Subsonic and intersonic range $0 \le v \le c_L$ ($c_3 = \sqrt{2}\, c_S$).

order to account for the nonlocality of atomic interactions, which has a significant effect in the core due to high gradients. We conjecture that nonlocal effects in the interface law cause instantaneous information transmission along the slip plane, thereby allowing *supersonic* dislocation motion. We extend model 1 to include a simpler but related alternative to nonlocal effects. We let the interface potential be given by $\Phi(u) + (\bar{\lambda}/2)(u')^2$, so that it depends on the slip displacement gradient u' in addition to u; here $\bar{\lambda}$ is a gradient coefficient. The interface law takes the form $\sigma = f(u) + \bar{\alpha}\dot{u} - \bar{\lambda}u''$, with $f(u) = \Phi'(u)$. The corresponding augmented version of (1) is

$$\frac{\mu}{\pi}A(v)\int_{-\infty}^{\infty}\frac{u'(z)}{z-x}\,dz + \mu B_\alpha(v)u' + \bar{\lambda}u'' + \sigma_{\rm appl} = f(u)\,, \qquad (12)$$

with B_α given by (7). Solutions $u(x)$ are subject to (3). An explicit solution of (12) is unlikely with $f(u)$ given by (8). We replace (8) by a b-periodic sawtooth function [17] satisfying

$$f(u) = 2\sigma_{\rm th}[u/b - H(u/b - 1/2)], \qquad 0 \le u < b\,; \qquad (13)$$

H is the step function. Using Fourier transforms in (12), and invoking (6), which remains valid with B_α from (7) in place of B, we obtain

$$\sigma_{\rm appl}(v) = \sigma_{\rm th}B_\alpha(v) \times \int_0^\infty \frac{(2/\pi)\,d\xi}{[1 + A(v)\xi + \lambda\xi^2]^2 + [B_\alpha(v)\xi]^2}\,, \qquad (14)$$

where $\lambda = 2\bar{\lambda}\sigma_{\rm th}/\mu^2 b$ is a nondimensional gradient coefficient [18]. The kinetic relation (14) for model 2 is shown in Fig. 2. At fixed v, $\sigma_{\rm appl}$ depends decreasingly on the gradient coefficient λ [Fig. 2(a)] and increasingly on the viscosity α [Fig. 2(b)]. The subsonic branch of $\sigma_{\rm appl}(v)$ exhibits a drag-dominated regime, nearly linear up to $0.5c_S$ for a wide range of λ values [14]. Then $d\sigma_{\rm appl}/dv$ increases due to relativistic effects; it remains positive for speeds beyond the Rayleigh speed c_R, in contrast to the situation in model 1. This stabilization is due to gradient effects.

The intersonic branch of $\sigma_{\rm appl}(v)$ is somewhat similar to the one predicted by model 1. It has a single minimum at a speed v_* depending on α and λ. Stable intersonic motion occurs for $\sigma_{\rm appl}$ above the critical value $\sigma_{\rm trans} = \sigma_{\rm appl}(v_*)$ at speeds $v > v_*$, since for $c_S < v < v_*$ $d\sigma_{\rm appl}/dv < 0$ and motion is unstable. For small viscosity α, v_* is slightly below $\sqrt{2}\,c_S$, while $\sigma_{\rm trans} = O(\alpha)$. In contrast to model 1, as $v \to c_L$, $\sigma_{\rm appl}(v)$ increases to a value $\sigma_{\rm sup} = \sigma_{\rm appl}(c_L)$ *below* $\sigma_{\rm th}$ in the presence of gradient effects ($\lambda > 0$).

Supersonic motion occurs above the critical stress level $\sigma_{\rm sup} = \sigma_{\rm appl}(c_L)$. For $v \ge c_L$, Eq. (14) simplifies to

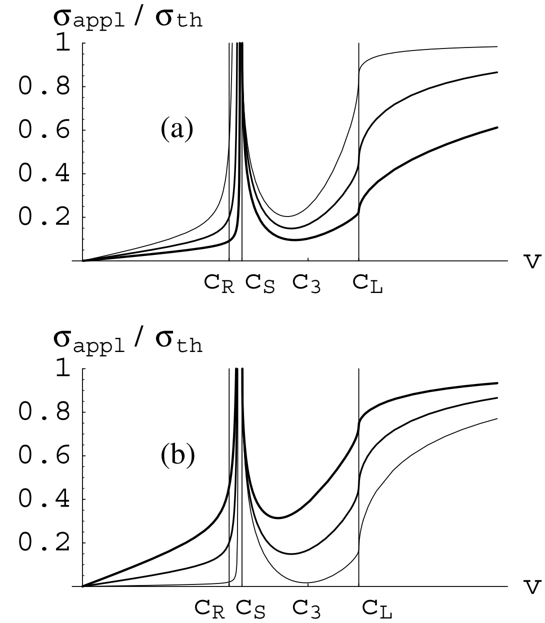

FIG. 2. The kinetic relation of model 2, $\sigma_{\rm appl}/\sigma_{\rm th}$ versus v from Eq. (14) ($c_3 = \sqrt{2}\,c_S$): (a) for viscosity $\alpha = 0.02$ and different values of the gradient coefficient, $\lambda = 0.02$, 0.2, 1, shown thicker for higher λ; (b) for different values of viscosity, $\alpha = 0.02$, 0.2, 0.5, and $\lambda = 0.2$, shown thicker for higher α.

$$\sigma_{\rm appl}(v) = \sigma_{\rm th}B_\alpha(v)/[4\lambda + B_\alpha^2(v)]^{1/2}. \qquad (15)$$

When $\lambda = 0$, $\sigma_{\rm appl}(v) = \sigma_{\rm th}$ for $v \ge c_L$ as in model 1. For $\lambda > 0$, $\sigma_{\rm appl}(v)$ is below $\sigma_{\rm th}$ and monotone increasing [19]; supersonic motion is stable.

According to model 2, steady motion can be subsonic only for $\sigma_{\rm appl}$ below $\sigma_{\rm trans}$. Above $\sigma_{\rm trans}$, a steadily moving dislocation has two speed choices: one subsonic and one intersonic (or supersonic for $\sigma_{\rm appl} > \sigma_{\rm sup}$).

Since $\sigma_{\rm appl}$ approaches $\sigma_{\rm th}$ for speeds slightly below c_S, the question arises whether an initially subsonic dislocation can ever exceed c_S. When impacted by a shock wave raising the stress above $\sigma_{\rm trans}$, a dislocation behaves in a highly transient manner, and need not follow the subsonic branch of the kinetic relation, valid only for *steady* motion; it is plausible that it will suddenly jump from the subsonic branch to the stable intersonic one. Another possibility, observed in the atomistic simulations of Gumbsch and Gao [4], is that dislocations nucleating under high enough stress immediately travel intersonically.

For a *screw* dislocation, model 2 yields a *monotone* kinetic relation, with $\sigma_{\rm appl}$ *below* $\sigma_{\rm th}$ even for $v > c_S$, in agreement with simulations [6]. For $v > 0.5c_S$ (including supersonic speeds) this relation resembles one obtained by Celli and Flytzanis [20] from a discrete model. Nonlocality in model 2 seems to capture some of the effects of discreteness in allowing supersonic motion.

Our predictions agree with atomistic simulations of Gumbsch and Gao [4], who report subsonic dislocation motion at or below an applied homogeneous shear strain $\varepsilon = 0.03$, intersonic motion for $0.035 \le \varepsilon \le 0.07$, and

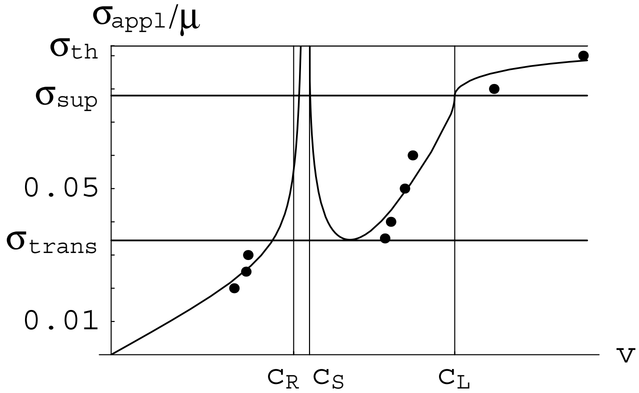

FIG. 3. Comparison of the kinetic relation of model 2 with the data of [4] (heavy points). Solid curve: $\sigma_{\mathrm{appl}}/\mu$ versus v from Eq. (14) for the fitting parameters $\sigma_{\mathrm{th}} = 0.093\mu$, $\alpha = 0.59$, $\lambda = 0.13$.

supersonic motion for $\varepsilon \geq 0.08$. Lacking estimates of the interface-law constants σ_{th}/μ, $\alpha = \bar{\alpha} c_S/\mu$, and $\lambda = 2\bar{\lambda}\sigma_{\mathrm{th}}/\mu^2 b$ for the model system of [4], we used them as fitting parameters in a numerical least-squares fit of (14) to those data of [4] that were reported to correspond to nearly uniform (stable) dislocation motion. This procedure yielded $\sigma_{\mathrm{th}} = 0.093\mu$, $\alpha = 0.59$, and $\lambda = 0.13$ [21]. Equation (14) for these values, plotted together with the data of [4], is shown in Fig. 3. The linear elasticity of the Peierls model dictates that $\sigma_{\mathrm{appl}} = \mu\varepsilon$. The data in Ref. [4] then imply that σ_{trans} lies in the range 0.03μ–0.035μ, and σ_{sup} in the range 0.07μ–0.08μ. Equation (14) predicts $\sigma_{\mathrm{trans}} = 0.034\mu$ and $\sigma_{\mathrm{sup}} = 0.078\mu$, within these ranges. In [4], dislocations with initial intersonic speeds of $1.25c_S$ to $1.15c_S$ were reported to move unsteadily. Similarly, model 2 predicts a critical speed $v_* = 1.2c_S$ below which intersonic motion is unstable. These dislocations were subject to stresses of 0.03μ or less (below the predicted value $\sigma_{\mathrm{trans}} = 0.034\mu$) and eventually slowed down to subsonic speeds.

In view of the highly approximate nature of the augmented Peierls model and the lack of estimates for the interface-law parameters [21], the above comparison is meant to illustrate only the qualitative agreement between Eq. (14) and the results of [4]. As is clear from Fig. 2, the general form of $\sigma_{\mathrm{appl}}(v)/\sigma_{\mathrm{th}}$ is the same for a wide range of α and λ values. Hence the prediction of intersonic and supersonic motion at high stress is parameter independent, and provides theoretical evidence that such processes are possible in crystalline solids under severe loads.

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