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Self-Oscillating Regime of Crack Propagation Induced by a Local Phase Transition at Its Tip

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We report an analytical study of propagation of a straight crack with a stress-induced local phase transition at the tip. We obtain its contribution to the dynamic fracture energy in explicit form and demonstrate that it nonmonotonically depends upon the crack tip velocity. We show that its descending part gives rise to the instability of the steady propagation regime. We obtain the dynamic phase diagram and indicate those domains where self-oscillating regimes of the crack motion take place.

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Unstable growth of cracks in the form of a stick-slip motion has long been observed in many materials including glasses, ceramics, and brittle polymers [1]. In linear elastic fracture mechanics (LEFM) this type of motion was attributed to a decrease in the resistance of solids to the crack growth manifested as a negative derivative of the velocity-dependent fracture energy $d\Gamma(v)/dv < 0$. It is generally accepted that this is related to some nonlinear processes localized in the vicinity of the crack tip (referred to as a "process zone") and essentially depends upon the zone properties. Various mechanisms have been discussed as candidates responsible for this phenomenon (such as molecular relaxation, transition from isothermal to adiabatic regime, crystallization at the crack tip, and microplasticity, [1,2]) though most of these are on a qualitative level, while efforts to mathematically treat microplasticity-based models resulted in the conclusion that they are intrinsically ill-posed [3].

During the last two decades experimental techniques to study rapid crack propagation have been greatly improved and applied to a number of materials [4,5]. The similarity of dynamic fracture behavior of materials with different microstructures such as brittle polymers, glasses, and some crystals gave rise to a hope that all of them may be described by a universal approach. It motivated devising several phase-field models [6] capable of reproducing microbranching and oscillatory instabilities of straight cracks, as those reported in [5].

Recently it was assumed [7] that the characteristic length scale associated with the distance on which crack profile deviates from LEFM is much larger than the scales due to any dissipative mechanisms. The results of the weakly nonlinear model turned out to be in quantitative agreement with data obtained in brittle gels [8].

One can attribute the nonlinearity accounted for in the paper [8] to acoustic phonons. In solids with nonprimitive lattice cells nonlinearity of nonacoustic degrees of freedom (e.g., related to optical phonons) may take place. If this happens, it becomes responsible for deviating from predictions of LEFM. This can result in phase transitions (PTs) localized in the vicinity of the crack tip referred to here as "local phase transitions" (LPTs) providing a natural emergence of the characteristic scale.

The LPT phenomenon attracted attention since late 1970s, being a key mechanism responsible for the effect of the LPT-related improvement of strength observed in ZrO_2-based ceramics and in some steels [9]. Observations of LPTs at tips of cracks have also been reported for some other inorganic solids: it has been observed during fracture of metals (cf. Figure 1 of Ref. [10]) and in ferroelectrics [11]. Besides LPT was observed in resins [12] and recently LPTs following fracture of polymers have been reported [13]. The LPT effect on the dynamics of cracks has not been addressed so far.

In this Letter for the first time we describe a physical mechanism responsible for the nonmonotonicity of $\Gamma = \Gamma(v)$ related to LPT at the crack tip, and resulting in self-oscillations during its propagation. We show that LPT gives rise to a configurational viscous friction force resisting the crack motion. It exhibits a descending behavior

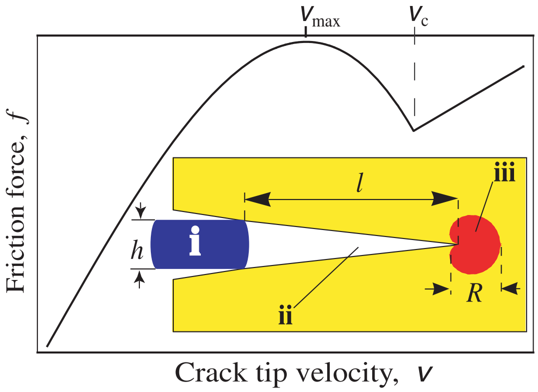

FIG. 1 (color online). Dependence of the force, resisting the crack motion upon the velocity of the crack tip v exhibits maximum at $v = v_{\max}$ and gives rise to the descending part at $v_{\max} \le v \le v_c$. Inset shows the sketch of wedging: (i) the wedge, (ii) the crack, and (iii) the region where the LPT is localized.

within a certain range of crack velocities and gives rise to self-oscillatory regimes of crack propagation.

In order to describe LPT one can introduce the order parameter field η where value $\eta = 0$ corresponds to the bulk phase away from the crack tip, while the distribution $\eta(r, t) \neq 0$, $\eta(\infty, t) = 0$ accounts for a new state localized at the crack tip. This field can be described within the Landau theory of PTs [14] and obeys the generalized Ginzburg-Landau-Khalatnikov equation [15]:

$$\kappa \frac{\partial \eta}{\partial t} = g \Delta \eta - \left\{ \alpha - \frac{4A(1-2\nu)(1+\nu)}{E} \sigma_{ii}(\mathbf{r}, t) \right\} \eta - \beta \eta^3 - \gamma \eta^5, \tag{1}$$

where the striction interaction between an inhomogeneous stress and the order parameter field is accounted for: $A > 0$ is the striction constant, α, β, $\gamma > 0$, $\kappa > 0$ and $g > 0$ are constants and E is the Young's modulus, ν is the Poisson's ratio, $\sigma_{ij}(r, t)$ is the stress tensor. Equation (1) describes both the case of the second order LPT at $\beta > 0$ as well as that of the first order close to the second order transition at $\beta < 0$.

In the case of a plane, normally loaded crack considered here the stress tensor has the trace $\sigma_{ii}(\mathbf{r}, t) = 2K_I \cos(\theta/2)/(2\pi r)^{1/2}$, where K_I is the dynamic stress intensity factor (SIF). We consider further a moving frame; thus, $r = \{(x - vt)^2 + y^2\}^{1/2}$ is the distance and θ is the angle counted off from the tip of the crack moving with the velocity v along Ox. It has been shown that the bifurcation of Eq. (1) with emerging of a nonzero solution takes place at $\alpha \leq \alpha_* > 0$ [10]:

$$\alpha_* = \alpha_*^{(0)} + \delta - \frac{\kappa^2 v^2}{4g}; \qquad \alpha_*^{(0)} = \left(\frac{4}{\pi^2 g}\right)^{1/3} \left[\frac{AK_I(1-2\nu)(1+\nu)}{E}\right]^{4/3}. \tag{2}$$

Here, $\alpha_*^{(0)} + \delta > 0$ is the bifurcation point in the case of the motionless crack, $\delta = 0$ at $\beta > 0$ and $\delta = 3\beta^2 s_4^2/16\gamma s_2 s_6$ at $\beta \leq 0$, where $s_n = \int \psi^n(\mathbf{r}) dx dy$. The bifurcation represents a transformation of the trivial solution $\eta \equiv 0$ of (1) stable at $\alpha > \alpha_* + \delta$, into the nontrivial one:

$$\eta(\mathbf{r}) \approx \xi \psi(\mathbf{r}); \qquad \psi(\mathbf{r}) = \exp\left\{ -\frac{\kappa v r \cos(\theta)}{2g} - \frac{r}{\sqrt[3]{4R}} + \sqrt[3]{4}\left(\frac{r}{R}\right)^{1/2} \cos(\theta/2) \right\}, \tag{3}$$

$$\xi^2(v) = \frac{-\beta s_4 + \{\beta^2 s_4^2 + 4\gamma[\alpha_*(v) - \alpha] s_2 s_6\}^{1/2}}{4\gamma s_6} \tag{4}$$

describing the LPT. The latter perturbs the strain field, ε_{jk}, around the crack tip:

$$\varepsilon_{jk} = \varepsilon_{jk}^{(0)} + A \int G_{jl}(q) q_l q_k Q(q) \exp(iqr) \frac{d^3 q}{(2\pi)^3}, \tag{5}$$

where $\varepsilon_{jk}^{(0)}$ is the strain field at the crack tip without LPT, q is the wave vector, $G_{jk}(q)$ is the Fourier-transform of the elastic Green function of the solid, $Q(q)$ is the Fourier transform of η^2: $Q(q) = \int \eta^2(r) \exp(iqr) d^3 r$. The solution (3) and (5), is stable at $\alpha \leq \alpha_* + \delta$. The size

$$R \sim (Eg/AK_*)^{2/3} \tag{6}$$

representing the LPT region establishes the characteristic scale of the process zone in our approach. Here K_* is the SIF corresponding to the bifurcation point. A detailed derivation of Eq. (2) and (3) can be found in [10,16].

Equation of motion (1) may be obtained by using the standard Ginzburg-Landau free energy together with the dissipative function (per unit crack front length):

$$D = \frac{\kappa}{2} \int \left(\frac{\partial \eta}{\partial t}\right)^2 dx dy \tag{7}$$

[17], the integration in (7) runs over the whole area of the (x, y) plane.

The rate of the free energy, dF/dt, is the power of the energy losses due to LPT. If it admits representation in the form $dF/dt = f_{\mathrm{LPT}} \times v$, the factor f_{LPT} has the meaning of a configurational friction force acting on the crack tip. Using a well-known relation of the power of losses to the dissipative function $dF/dt = -2D$ [17], substituting the solution (3) into (7) one finds after integration $f_{\mathrm{LPT}} \sim J\kappa\xi^2 v$. Here $J = \int (\partial\psi/\partial x)^2 dx dy$. Our numerical calculation shows that at $v < v_c$ the dependence of J upon v is weak and is accurately approximated by a constant $J \approx 5$. Here, v_c is the characteristic velocity

$$v_c = \frac{2(g\alpha_*^{(0)})^{1/2}}{\kappa} \sim \frac{R}{\tau_c}; \qquad \tau_c = \frac{\kappa}{\alpha_*^{(0)}} \tag{8}$$

and τ_c is the characteristic LPT time. The proportionality $f_{\mathrm{LPT}} \sim v$ indicates the viscouslike character of this force. The total friction force has the form $f = kv + f_{\mathrm{LPT}}$, where k is a constant. By the addition of the term kv, we phenomenologically account for other linear dissipation mechanisms different from LPT. One finds

$$f = \begin{cases} kv, & \alpha > \alpha_* + \delta \\ kv + J\kappa\xi^2 v, & \alpha \leq \alpha_* + \delta \end{cases}. \tag{9}$$

The second term of the lower line of (9) represents the contribution to the friction force of the energy dissipation within the LPT zone.

The amplitude ξ depends upon the crack tip velocity $\xi = \xi(v)$; hence, the friction force f nonlinearly depends upon it. At $v = v_c$ the crack moves so fast that the material in front of it has no time to transform into the phase $\eta(\mathbf{r}) \neq 0$. The amplitude, therefore, vanishes at $v \to v_c$

and at $v \geq v_c$ only the linear contribution $f = kv$ to the friction force survives.

From here on we illustrate the $f = f(v)$ dependence within the case of the second order LPT ($\beta > 0$, $\xi^2 = (\alpha_* - \alpha)s_2/\beta s_4$) admitting a simple analytical solution. At $\alpha \leq \alpha_*$ the function $f(v)$ (9) exhibits a maximum at $v^2_{\max} = 4g\{k\beta s_4 + J\kappa(\alpha^{(0)}_* - \alpha)s_2\}/3J\kappa^3$. The inequality $v_{\max} < v_c$ holds, if $k < J\kappa(\alpha + \alpha^{(0)}_*)s_2/\beta s_4$. This condition corresponds to our assumption of the domination of the LPT friction mechanism. Under this condition, therefore, the friction force exhibits the descending part at the velocities within the interval $v_{\max} < v < v_c$ (Fig. 1). It is in this interval the stick-slip instability takes place. Such a behavior holds also in the first order LPT case.

We demonstrate this within the example of a wedge-loaded crack (inset of Fig. 1) first analyzed in [18]. Wedging is a special case of the double cantilever beam (DCB) configuration studied later in [19,20]. It has been shown that the DCB configuration possesses inertia, and the corresponding equation of the crack tip motion has the second time derivative [18–20]. Using original notations of the paper [18] one finds

$$m\frac{d^2l}{dt^2} = \left(1 - \frac{v}{v_R}\right)\frac{(1-\nu^2)K_I^2}{E} - \Gamma(v). \tag{10}$$

Here $l = l(t)$ is the crack length in front of the wedge, the dynamic SIF, $K_I = K_I(l)$, is defined by the thin wedge (thickness h) [18]. Here $\Gamma(v) = 2\gamma + f(v)$ is the dynamic fracture energy, γ is the surface energy, m is the associated crack mass [18], v_R is the Rayleigh velocity, and the factor $(1 - v/v_R)$ accounts for the dynamic SIF [20], the friction force, $f(v)$, obeys (9). For simplicity we only consider the rectilinear crack tip movement.

Assume the velocity composed of the constant wedge velocity, V, and the speed of the crack tip with respect to the wedge, dl/dt, as $v = V + dl/dt$. By L we denote the crack length during the steady motion $dl/dt = 0$. During the unsteady motion we represent the crack length as $l(\tau) = L[1 + z(\tau)]$, where $\tau = (q/m)^{1/2}t/L$ is dimensionless time, z is the dimensionless length and $q = Eh^2/2\pi(1-\nu^2)$. Equation (10) with the friction force (9) can be rewritten in the following form:

$$z'' + z = F(z, z'), \tag{11}$$

where we denote $z' \equiv dz/d\tau$ and $z'' \equiv d^2z/d\tau^2$, and the function $F(z, z')$ contains all the rest of the terms in (10). The explicit form of this lengthy function will be given in full in the forthcoming paper. One can treat (11) as a quasilinear equation, provided $z, z' \ll 1$ (which is assumed here). In this case the van der Pol approach [21] can be applied for its analysis. Within this approach, the solution of Eq. (11) is found in the form $z(\tau) = \rho\cos(\tau - \varphi)$ where the amplitude $\rho = \rho(\tau) > 0$ obeys the following equation:

$$\frac{d\rho}{d\tau} = \Phi(\rho) = -\frac{1}{2\pi}\int_0^{2\pi} F(\rho\cos\zeta, -\rho\sin\zeta)\sin\zeta d\zeta. \tag{12}$$

We report the analysis of the case $v \ll v_R$. Integration in (12) yields

$$\Phi = -\frac{0.5L}{(mq)^{1/2}} \times \begin{cases} k\rho, & \alpha > \alpha^{(0)}_* - \kappa^2 v^2/4g \\ \frac{J\kappa L}{\beta}(Q_1\rho - Q_2\rho^2 + Q_3\rho^3), & \alpha < \alpha^{(0)}_* - \kappa^2 v^2/4g \end{cases}, \tag{13}$$

where $\alpha^{(0)}_* = \{A(1-2\nu)h/\pi(1-\nu)\}^{4/3}g^{-1/3}L^{-2/3}$, $Q_1 \approx \alpha^{(0)}_* - \alpha - 3\kappa^2V^2/4g + k\beta/kJ$, $Q_2 \approx 0.018\alpha^{(0)}_*$, and $Q_3 \approx 0.2(\alpha^{(0)}_* - 0.94q\kappa^2/gm)$.

Equation (12) and (13) is one dimensional, and its analysis reduces to the enumeration of its fixed points: the one at $\rho = 0$ is interpreted as a focus in (z, z') plane, while those at $\rho \neq 0$ as cycles [21]. This enables one to attribute various regimes of the crack growth to domains of the phase diagram on the plane (α, V). One of the phase diagrams for this system is shown in Fig. 2, while the whole set of diagrams will be given in detail in the forthcoming paper.

At $\alpha > \alpha_*$ (where $\alpha_* = \alpha^{(0)}_* - \kappa^2V^2/4g$ is shown in Fig. 2 by the solid line) the phase $\eta \equiv 0$ is stable everywhere in the solid. In this region $\Phi \sim -\rho$ is given by the first expression (13) and (12) yields a single attractive fixed point $\rho = 0$ interpreted as the attractive focus in (z, z') plane (Fig. 2, inset a). Any perturbation of the crack length therefore vanishes with time and $l(\tau) \to L$; hence, the crack tip propagation is steady.

In contrast, if $\alpha < \alpha_*$, on both sides of the line $\alpha = \alpha_1 = k\beta/J\kappa + \alpha^{(0)}_* - 3\kappa^2V^2/4g$ (shown by the dashed line) regimes with cycles in the (z, z') plane take place. The region to the right of this line is characterized by a single stable cycle (shown in the inset b), while the phase portrait in the region to its left exhibits attractive focus in the origin surrounded by unstable internal and stable external cycles (inset c). In this regime small perturbations of the crack length vanish, while larger ones grow and reach the self-oscillating regime corresponding to the attractive cycle. At $\alpha < \alpha_*$ and $\alpha < \alpha_2 = \alpha_1 - 0.002(\alpha^{(0)}_*)^2/Q_3$ a steady regime of crack motion returns (inset d).

Defining a complete set of brittle materials where the LPT takes place is beyond the scope of this Letter. Below we make estimates of parameters of our approach within several examples of crystals exhibiting bulk structural PTs to which the LPT description certainly applies. Structural PTs are divided into the order-disorder and displacive classes. For the order-disorder class of PTs the kinetic

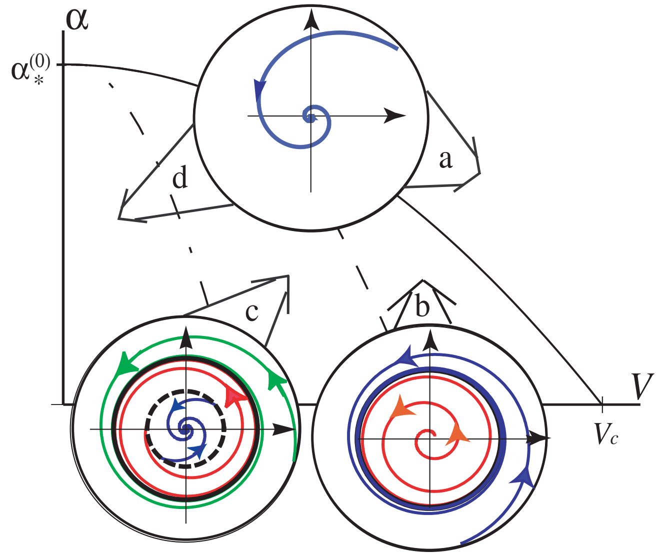

FIG. 2 (color online). Dynamic phase diagram in (V, α) plane: the solid line $\alpha = \alpha_*$ separates the region with no phase transition at the crack tip from those with LPT. The dashed and dashed-dotted lines α_1 and α_2 separate the regions corresponding to different regimes of the crack motion. Insets show the corresponding phase portraits in the (z, z') plane: foci (a) and (d) correspond to the steady crack propagation, while the phase portraits with cycles (b) and (c) describe various self-oscillating regimes.

factor κ can take the value of $\kappa \sim 10^{-7}$ s as in the case of $\mathrm{AgNa(NO_2)_2}$, $\kappa \sim 10^{-11}$ s as in $\mathrm{KNO_3}$ or $\mathrm{NaNO_2}$ up to $\kappa \sim 10^{-12}$ s as in the Rochelle Salt, triglycine sulfate and $\mathrm{KD_2PO_4}$. In all materials of this class $g \sim 10^{-15}$ cm^2 and $A \sim 10$ to 10^2 [22,23]. In the case of materials exhibiting displacive structural PTs (such as $\mathrm{BaTiO_3}$, $\mathrm{PbTiO_3}$, $\mathrm{Pb(Ti_x, Zi_{1-x})O_3}$, $\mathrm{SrTiO_3}$ and many others) one finds $g \sim 10^{-14}$ cm^2, $\kappa \sim 10^{-13}$ s and $A \sim 10^{-1}$ to 1 [22]. Assume $K_* \approx K_{\mathrm{IC}}$. For inorganic materials one can estimate $K_* \approx K_{\mathrm{IC}} \sim 10^7$ erg/cm$^{5/2}$ (as in the case of $\mathrm{BaTiO_3}$) up to $K_{\mathrm{IC}} \sim 10^8$ erg/cm$^{5/2}$ (as in $\mathrm{PbTiO_3}$ and $\mathrm{Pb(Ti_x, Zi_{1-x})O_3}$) [24]. In all these materials the Young's modulus, E, and the mass density, ρ, can be estimated as $E \sim 10^{12}$ erg/cm^3 and $\rho \sim 10$ g/cm^3.

Making use of these parameters and (2) the ratio of the characteristic velocity, v_c, (8) to the Rayleigh velocity, $v_R \approx (0.85\text{–}0.95)(E/\rho)^{1/2}$:

$$\frac{v_c}{v_R} \sim \left(\frac{\rho}{E}\right)^{1/2}\left(\frac{AK_*}{E}\right)^{2/3}\frac{g^{1/3}}{\kappa} \qquad (14)$$

can be estimated as $v_c/v_R \sim 10^{-6}$ to 1 in the case of the order-disorder PTs and $v_c/v_R \sim 0.1$ to 1 in the case of PTs of the displacive class. Thus, in solids with order-disorder transitions the characteristic velocity may be small and only slow cracks may exhibit the stick-slip behavior. In contrast, the LPT-driven instability takes place for fast cracks for solids exhibiting PTs of the displacive type.

In the case of the order-disorder PTs one finds the zone size (6) $R \sim 0.1$ to 1 nm. The same estimate for the displacive PTs yields $R \sim 1$ to 10 nm.

The constant α of Eq. (1) can be represented as $\alpha = a(T - T_c)$, where T is the temperature and T_c is the Curie temperature. The constant a is known to have the same order of magnitude $a \sim 10^{-5}$ K^{-1} for a vast number of solids (such as $\mathrm{BaTiO_3}$, $\mathrm{PbTiO_3}$, $\mathrm{Pb(Ti_x, Zi_{1-x})O_3}$, $\mathrm{SrTiO_3}$, $\mathrm{KNO_3}$, $\mathrm{LiTaO_3}$, $\mathrm{LiNbO_3}$ and many others [23,25]). Making use of (2) one can estimate the difference, $\Delta T = T_* - T_c$, between the temperature, T_*, at which the bifurcation takes place and the Curie temperature: $\Delta T \sim (AK_*)^{4/3}/(ag^{1/3}E^{4/3})$. One finds $\Delta T \sim 10^3$ K to 10^4 K. This implies that formation of the LPT practically always follows fracture in such materials. Indeed, the observation of LPT following fracture in $\mathrm{Pb(Ti_x, Zi_{1-x})O_3}$ has been reported [11]. This seems to contradict to the rarity of the reported cases of the LPTs observations. The reason is that (i) the LPT can only be explicitly observed at the tip of a loaded crack and disappears with its unloading and (ii) the zone size, R, is beyond the optical limit. This caused the LPT being only noticed, if the long-living metastable trace (forming behind the propagating LPT) was detected on the fracture surfaces as in the cases of $\mathrm{ZrO_2}$ [9] and $\mathrm{Pb(Ti_x, Zi_{1-x})O_3}$ [11]. For most PTs, however, either the metastable trace has a short lifetime and decays before the observation, or it does not form at all.

The dimensionless ratio $r = (Ef_{\mathrm{LPT}})^{1/2}/K_{\mathrm{IC}}$ determines the relative contribution of the LPT to the dynamic fracture resistance. To estimate r we use the expression (9) for the force assuming $k = 0$ and $v \sim v_c$. In the case of the first-order transitions the amplitude ξ can be estimated by its jump in the transition point: $\xi^2 \approx -\beta s_4/\gamma s_6$. The ratio s_4/s_6 we obtained numerically to vary from 0.2 to 0.8 with the crack velocity variation from zero to v_c. We make this estimate for three perovskites $\mathrm{BaTiO_3}$, $\mathrm{PbTiO_3}$ and $\mathrm{Pb(Ti_x, Zi_{1-x})O_3}$. In the former case $\beta \sim -10^{-13}$ cm^3/erg < 0 and $\gamma \sim 10^{-22}$ cm^6/erg, while in the both latter cases $\beta \sim -10^{-13}$ cm^3/erg < 0 and $\gamma \sim 10^{-24}$ cm^6/erg [25]. This yields $r \sim 0.1$ for $\mathrm{PbTiO_3}$ and $\mathrm{Pb(Ti_x, Zi_{1-x})O_3}$ and $r \sim 1$ for $\mathrm{BaTiO_3}$. The high values of r indicate that the effect is important and should manifest itself in a considerable part of the phase diagram.

To summarize, in solids with nonprimitive crystal cell stress-induced local phase transitions may take place at the crack tip. Their crucial role in the crack dynamics is due to their contributions to the velocity-dependent resistance to fracture. We explicitly calculated the viscous friction force due to the local phase transition and showed that it provides self-oscillating behavior of the crack tip motion within certain domains of the dynamic phase diagram.

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