Dynamic instability of dislocations due to nucleation of a new phase

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Dislocation lines in a crystal close to a bulk phase transition can be coated by nuclei of a new phase which for a moving dislocation gives rise to a viscous friction force. In some range of the material parameters this force leads to a dynamic instability of the defect line, resulting from an intricate interplay between the shape fluctuations of the defect and the amplitude fluctuations of the nucleus. The instability shows up in the linear response of the dislocation to a periodic change of the driving force and in the structure factor of the order-parameter fluctuations of the nucleus.

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In a crystal, undergoing some bulk phase transition, the elastic distortion field around a dislocation induces a corresponding inhomogeneous distribution of local transition temperatures. As a consequence, dislocations close to the transition point of the reference crystal can be coated by nuclei of a globally unstable phase [1–4]. For a moving dislocation, the continuous dissipation of energy into the attendant nucleus generates a viscous-friction force [5]. If the transition is of first order, an additional dry-friction force appears in the hysteresis temperature range due to phase transformation into a metastable trail behind the defect [5]. Until recently, however, these phenomena have only been discussed for straight dislocation lines moving at a constant velocity [6], disregarding implications of line- and order-parameter fluctuations.

Allowing such effects, we have recently shown [7] that, in a regime where a Peierls stress [8] and an inertial term [9] can be neglected, the glide motion of a dislocation close to a first-order phase transition obeys a Kardar-Parisi-Zhang (KPZ) equation [10], supplemented by a dry-friction force. In Ref. [7] it was argued that, due to the competition between the KPZ nonlinearity and the dry-friction term, the dislocation line develops a zigzaglike roughening behavior. An additional nucleus-induced viscous-friction force has also been taken into account, but assumed to simply renormalize the bare mobility coefficient of the dislocation.

In the present paper we will show that in some range of the material parameters the viscous-friction term alone gives rise to a shape instability of the dislocation line which is totally different from the previously discussed roughening instability. Whereas the latter evolves from local changes of the slope of the line (relative to the Burgers vector), the new instability is initiated by local velocity fluctuations (which simultaneously involve curvature fluctuations). In fact, due to a finite relaxation time for readjustments of the nucleus, a local acceleration of the defect reduces the nucleus amplitude, and consequently lowers the strength of the viscous-friction force. This in turn generates an increase of the local defect velocity which then proliferates in a self-amplifying way. Opposite to this, the line tension tries to stretch the defect, and, competing with the former effect, excites an oscillation of the dislocation line at the instability threshold.

The phenomenon is most easily seen in the linear response function of the defect line to a periodic change of the Peach-Köhler force [11] driving the glide motion of the dislocation. It also shows up in the structure factor of the order-parameter fluctuations of the nucleus. A simple way to observe these quantities without interference by the previously discussed [7] roughening mechanism is to avoid the hysteresis temperature range or, alternatively, to consider the case of a second-order transition. We here focus on the more transparent analysis of the second scenario, although the results are expected to apply as well to weakly first-order transitions. For simplicity reasons our approach will also be restricted to the vicinity of the nucleation threshold in the globally stable high-symmetry phase.

Choosing the x,z plane as the glide plane, we describe the configurations of the dislocation line at time t by the Monge representation $z=h(x,t)$. Then the coupling to a scalar order-parameter field $\varphi(\boldsymbol{r},t)$ of a second-order phase transition is most easily described by the model Hamiltonian

$$H=\int dx\left[\frac{\sigma}{2}(\partial_x h)^2-kh\right]+\int d^3r\left[\frac{1}{2}(\nabla\varphi)^2+\frac{\varepsilon+U(h)}{2}\varphi^2+\frac{u}{4}\varphi^4\right], \qquad (1)$$

where σ means the line tension of the dislocation (see, e.g., Refs. [9] and [12]), k is the Peach-Köhler force [11], $\varepsilon=\alpha(T-T_c)$ measures the temperature distance from the critical point, and

$$U=\kappa\frac{b_z}{2\pi}\frac{1-2\nu}{1-\nu}\frac{y}{[z-Vt-h(x,t)]^2+y^2}. \qquad (2)$$

Up to a coupling constant κ the expression (2) represents the trace of the elastic strain field generated by a dislocation at

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position $z=Vt+h(x,t)$ where V is the mean velocity of the defect (to be determined later). The explicit form, given in Eq. (2), applies to an isotropic medium with Poisson ratio ν, and to a dislocation with the z component b_z of its Burgers vector (compare Ref. [7] where, however, the x,y plane has been chosen as the glide plane).

Since in the present context the KPZ nonlinearity is irrelevant, we can assume an Edwards-Wilkinson-like [13] process for h whereas for φ we adopt (as in Ref. [7]) a simple model-A-type [14] relaxation behavior. A convenient representation of this model for the subsequent analysis is the dynamic functional [15,16]

$$I=\int dtdx\,\tilde{h}[V+\partial_t h+B^{-1}\delta H/\delta h-B^{-1}\tilde{h}]$$
$$+\int dtd^3r\,\tilde{\varphi}[\partial_t\varphi+\lambda\,\delta H/\delta\varphi-\lambda\tilde{\varphi}] \tag{3}$$

where $\tilde{h},\tilde{\varphi}$ mean response fields [17], and B,λ are kinetic coefficients. From Eq. (3), e.g., the response function $\delta\langle h(x,t)\rangle/\delta k(x',t')$ can be generated via

$$\int D[h,\tilde{h},\varphi,\tilde{\varphi}]\,h(x,t)\tilde{h}(x',t')\exp\{-I[h,\tilde{h},\varphi,\tilde{\varphi}]\}$$
$$\equiv\langle h(x,t)\tilde{h}(x',t')\rangle$$
$$=B\,\delta\langle h(x,t)\rangle/\delta k(x',t'). \tag{4}$$

In order to eliminate the inconvenient h dependence in Eq. (2), we use the transformation $z\to\zeta\equiv z-Vt-h(x,t)$ which enforces the replacements $\partial_t\to\partial_t-(V+\partial_t h)\,\partial_\zeta$ and $\partial_x\to\partial_x-(\partial_x h)\partial_\zeta$. Neglecting the ''slope term'' $(\partial_x h)[2\partial_x-(\partial_x h)\partial_\zeta]\partial_\zeta$, this leads in the second integral of Eq. (3) to the appearance of the non-Hermitian ''Hamilton'' operator

$$\mathbf{H}\equiv-\partial_y^2-[\partial_\zeta+(2\lambda)^{-1}A]^2+U, \tag{5}$$

involving the imaginary ''vector potential'' $A\equiv V+\partial_t h-\lambda\partial_x^2 h$, and to a shift $\varepsilon\to\varepsilon+(4\alpha\lambda^2)^{-1}A^2$.

As observed in Ref. [18] in a similar situation, the right and left eigenfunctions ψ_ν^+,ψ_ν^- and the eigenvalues $-\varepsilon_\nu$ of $\mathbf{H}$ show the behavior $\psi_\nu^\pm(y,\zeta;A)=\psi_\nu(y,\zeta;0)\exp[\mp(2\lambda)^{-1}A\,\zeta]$, $\varepsilon_\nu(A)=\varepsilon_\nu(0)$. The set $\{\psi_\nu\}$ at $A=0$ consists of scattering states (for which ν is continuous), and of bound states, captured by the attractive section of the ''potential'' $U(y,\zeta)$ [19]. The bound-state wave functions are chosen to obey $(\psi_\mu,\psi_\nu)=\delta_{\mu\nu}$ where the scalar product means integration over the whole y,ζ plane.

Whereas the scattering states represent a convenient basis for the description of bulk fluctuations of the order parameter φ, the bound states form a natural support for the nucleus attached to the defect. For a static straight dislocation line the ground-state ''energy'' $\varepsilon_0=\alpha(T_0-T_c)$ defines the nucleation temperature T_0, close to which $\psi_0(y,\zeta)$ determines the order-parameter profile transverse to the defect line. When the dislocation moves with a constant velocity V, the nucleation threshold is shifted to $T_0(V)=T_0-(4\alpha\lambda^2)^{-1}V^2$, and the order-parameter profile deforms into $\psi_0^+(y,\zeta;V)$. At the critical velocity $V_c\equiv2\lambda\varepsilon_0^{1/2}$ the wave function ψ_0^+ becomes delocalized (as pointed out in Ref. [6] and, in a different context, in Ref. [18]), and $T_0(V_c)=T_c$.

Insertion of the spectral representation of $\mathbf{H}$ into the second integral of Eq. (3) suggests to introduce the projections $\chi_\nu(x,t)\equiv(\psi_\nu^-,\varphi)$, $\tilde{\chi}_\nu(x,t)\equiv(\tilde{\varphi},\psi_\nu^+)$ (where now the $\psi_\nu^\pm$ depend on A). Close to the nucleation threshold $\chi_0(x,t)$ describes the order-parameter amplitude of the nucleus along the dislocation line at time t. In case of uniform motion of a straight defect, χ_0 has a constant value $X(V)$ which, together with the velocity V, is approximately determined (as in Ref. [6]) by the saddle-point Eqs. (3).

In order to derive these equations explicitly, we use in the first integral of Eq. (3) the chain of identities

$$(\psi_0^+,[\partial_h U]\,\psi_0^+)=-(\psi_0^+,[\partial_\zeta U]\,\psi_0^+)$$
$$=2(\partial_\zeta\psi_0^+,U\psi_0^+)$$
$$=2\lambda^{-1}A\,(\partial_\zeta\psi_0^+,\partial_\zeta\psi_0^+)$$

where the last form is the only term which survives, after U has been expressed via Eq. (5). With regard to an expansion around V we will define $M(V)\equiv B^{-1}\lambda^{-1}(\partial_\zeta\psi_0^+,\partial_\zeta\psi_0^+)_{A=V}$. In the second integral of Eq. (3) we use the relation $(\psi_0^-,\mathbf{H}\,\psi_0^+)=-\varepsilon_0$, and the definitions $\tau(V)\equiv\varepsilon-\varepsilon_0+(2\lambda)^{-2}V^2=\alpha[T-T_0(V)]$, $S^{-1}(V)\equiv(\psi_0^-,\psi_0^{+3})_{A=V}$ where $S(V)$ measures the cross section of the nucleus.

With the notations $Y(V)\equiv VM(V)$ and $F\equiv k/B$ the resulting saddle-point equations for V and X read

$$V+X^2(T,V)Y(V)=F, \tag{6}$$

$$[S(V)\tau(T,V)+uX^2(T,V)]X(T,V)=0, \tag{7}$$

where the parametric dependences on T have been made explicit. Equation (7) describes the nucleation process as a sharp (mean-field) phase transition which in reality is smeared out by thermal fluctuations [20]. Nevertheless, $\langle\chi_0^2\rangle\approx X^2$ for $\tau^2\gg uS^{-1}(V)$ where $S(V)$ monotonically increases from $S(0)\propto\varepsilon_0^{-1}$ to $S(V_c)=\infty$. At the most dangerous point $V=0$ the condition reads $\tau^2\gg\varepsilon_G\varepsilon_0$ where $\varepsilon_G\propto u$ is the Lewanjuk-Ginzburg temperature interval of two-dimensional nonclassical behavior (see, e.g., Ref. [21]). Thus the saddle-point approximation becomes acceptable for systems close to the tricritical threshold $u=0$ of a first-order transition in the bulk (which is common in structural phase transitions).

The possible appearance of an instability already shows up in the isotherms $F=F(T,V)$ of Eq. (6) which below the classical nucleation threshold approximately are cubic parabulas [slightly deformed by the weak V dependence of the factor $M(V)S(V)$]. As illustrated in Fig. 1, there exists a critical isotherm $T=T_1$ which has a horizontal slope at the nucleation threshold $T=T_0(V)$. In fact, the intersection value V_1, defined by $T_0(V_1)=T_1$, will later be shown to generically obey $V_1<V_c$. For temperatures $T<T_1$ there appears a velocity interval where the isotherms display the un-

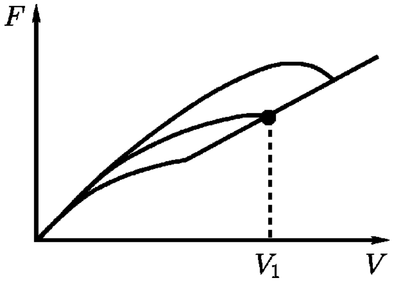

FIG. 1. F,V phase diagram, showing a stable, a critical, and an unstable isotherm (corresponding to the lower, the middle, and the upper curve). Outside the nucleation regime all isotherms collapse to the trivial line $F=V$.

stable behavior $F'(T,V)\equiv\partial_V F(T,V)<0$. The boundary $F'(T,V)=0$ defines a spinodal-like instability line $T=T_s(V)$ in the T,V ''phase diagram'' shown in Fig. 2.

We now take care of thermal noise and of shape fluctuations of the defect, caused by oscillations of the Peach-Köhler force. For $\tau^2\ll\varepsilon_1^2$ the resulting order-parameter fluctuations of the nucleus around, e.g., the positive root X of Eq. (7) are included in $\chi(x,t)\equiv\chi_0(x,t)-X$ and $\tilde{\chi}(x,t)\equiv\tilde{\chi}_0(x,t)$. An effective weight functional $\exp\{-J[\tilde{h},h,\tilde{\chi},\chi]\}$ can be obtained by integrating the corresponding weight with the full action (3) over the fields $\tilde{\chi}_\nu$, χ_ν with $\nu>0$. This can safely be done by perturbation theory, because in the spectrum of the eigenvalues these ''hard-mode'' fields are separated by a gap from the ground-state amplitude χ_0. Since, moreover, this procedure does not create dangereous fluctuations in χ, a tree approximation will be sufficient. Keeping track of the harmonic terms only, one finds, with the notation $X'\equiv\partial_V X$,

$$\begin{aligned} J=\int dt dx\{&\tilde{h}[(1+X^2Y')\partial_t h-(B^{-1}\sigma+\lambda X^2Y')\partial_x^2 h\\ &+2XY\chi-B^{-1}\tilde{h}]+\tilde{\chi}[\partial_t\chi-\lambda(\partial_x^2\chi+2\tau\chi)\\ &+2\lambda\tau X'(\partial_t h-\lambda\partial_x^2 h)-\Lambda\tilde{\chi}]\}. \end{aligned}\tag{8}$$

where $\Lambda(V)\equiv\lambda(\psi_0^-,\psi_0^-)_{A=V}$. The choice $X>0$, showing up in the coupling term of Eq. (8), has no effect on the quantities of interest which all depend on X^2 only.

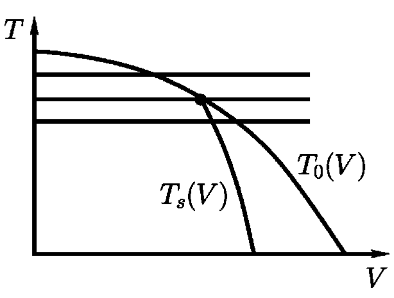

FIG. 2. T,V phase diagram, showing the isotherms of Fig. 1, the classical nucleation regime $T\leqslant T_0(V)$ and the spinoidal line $T=T_S(V)$.

The model (8) is a convenient basis for the discussion of Gaussian fluctuations around the mean-field behavior, presented in [6] and summarized in Ref. (6) and Ref. (7). It obeys the property of detailed balance only in the nucleus-free regime $X=0$, and in the more interesting case $V=0$ where also the pairs of variables $\tilde{h},h$ and $\tilde{\chi},\chi$ decouple. The coupling terms, arising for $V\neq0$ are responsible for the dynamic instability of interest which penetrates all correlation and response functions of the system. Anharmonic corrections to Eq. (8) will only be important for the saturation regime of the defect (reminding on the question of the late-stage behavior of spinodal decomposition).

In order to generate the set of correlation and response functions, one simply has to invert the kernel of the bilinear form composing the integrand of Eq. (8). The result for the spatial Fourier transform $R(q,t)$ of the response function $R(x,t)\equiv\langle h(x,t)\tilde{h}(0,0)\rangle$ in the hydrodynamic regime $q^2\ll|\tau|$ reads

$$R(q,t)=\Theta(t)\frac{1}{F'}\left[e^{-Dq^2t}-\left(1-\frac{\Delta}{2\lambda}\right)e^{-\Delta|\tau|t}\right].\tag{9}$$

Here, $\Theta(t)$ is the Heaviside step function, and

$$D\equiv\lambda+\frac{B^{-1}\sigma-\lambda}{F'},\quad \Delta\equiv\frac{2\lambda F'}{1+X^2Y'}.\tag{10}$$

The combinations $B^{-1}\sigma-\lambda$ and $1+X^2Y'$ both are positive which in the former case follows from a numerical estimate (given below), and in the latter case is obvious close to the nucleation threshold. Consequently, the two hydrodynamic modes appearing in Eq. (9) are stable below the spinodal line $T=T_s(V)$ where the stretching effect due to the line tension dominates. They both become unstable above the spinodal line where the self-amplifying acceleration effect, explained in the introduction, prevails. At the stability threshold $T=T_s(V)$ Eqs. (9) and (10) cease to be valid, and instead the stretching and acceleration mechanisms cooperate to produce, again for $q^2\ll|\tau|$, the damped oscillatory behavior

$$R(q,t)=\Theta(t)\frac{C}{B^{-1}\sigma-\lambda}\frac{1}{|q|}\sin(C|q|t)\,e^{-\Gamma q^2t}\tag{11}$$

(reminding on acoustic phonon excitations), with

$$C^2=2\lambda D\Delta|\tau|,\quad \Gamma\equiv\lambda+\frac{D\Delta}{4\lambda}.\tag{12}$$

Of course, the full crossover behavior between Eqs. (9) and Eq. (11) can also be extracted from (8).

Naturally, the above instability effects also enter the order-parameter fluctuations $S(x,t)\equiv\langle\chi(x,t)\chi(0,0)\rangle$. The corresponding structure factor is given by $S(q,\omega)=\lambda|G(q,\omega)|^2+B^{-1}|K(q,\omega)|^2$ where $G(x,t)\equiv\langle\chi(x,t)\tilde{\chi}(0,0)\rangle$, and $K(x,t)\equiv\langle\chi(x,t)\tilde{h}(0,0)\rangle$. In the regime $q^2\ll|\tau|$ it is convenient to normalize the contributions of both hydrodynamic modes such that their frequency integrals become equal to 1. This can be achieved by extracting an appropriate amplitude from each contribution which for the diffusion mode turns out to be smaller by a factor $q^2/|\tau|$. Neglecting therefore the diffusion part, one arrives at the result

$$S(q,\omega)=Q\,\frac{1}{\omega^2+[\Delta|\tau|]^2} \tag{13}$$

with

$$Q\equiv\Delta+B^{-1}\left(\frac{2\lambda X'}{1+X^2Y'}\right)^2|\tau|^2. \tag{14}$$

At $T=T_s(V)$ one finds

$$S(q,\omega)=\frac{Q}{4}\left[\frac{1}{(\omega+C|q|)^2+(\Gamma q^2)^2}+\frac{1}{(\omega-C|q|)^2+(\Gamma q^2)^2}\right], \tag{15}$$

i.e., the appearance of a Stokes and an anti-Stokes peak. One has to remember, of course, that Eqs. (13) and (15) only refer to the one-dimensional order-parameter fluctuations along the dislocation line.

We now demonstrate that for the behavior (9)–(15) there is a finite window in the parameter space of the model (6)–(8). The condition $T_0(V_1)=T_s(V_1)$ at first implies $V_1^2=2\lambda^2 uS^{-1}(V_1)M^{-1}(V_1)\approx 2\lambda^3 Bu$. Consequently, $V_1^2/V_c^2\approx\lambda Bu/\epsilon_0\approx 10^2\lambda Bu/\kappa^2$ where from Ref. [6] we have adopted the estimate $\varepsilon_0\propto 10^{-2}\kappa^2$. After insertion of the mean-field expression $\varphi^2(T=T_c)=-U/u$ into Eq. (1), we furthermore find $\delta^2 H/\delta U^2=-\Omega/(2u)$ (Ω meaning the volume), so that κ^2/u essentially measures the mean-field jump of the bulk modulus at T_c. Since this jump will at most be of the order of the shear modulus μ of the crystal (see, e.g., Ref. [12]), we obtain $V_1^2/V_c^2\approx 10^2\lambda B/\mu$. Insertion of the approximate values $\lambda\approx 10^{11}, B\approx 10^{-4}, \mu\approx 10^{11}$ in cgs units, adopted from Refs. [22] and [12], eventually leads to the result $V_1/V_c\approx 10^{-1}$ at least which confirms our earlier assertion. In Eq. (3) all lengths are measured in units of the lattice spacing a [due to the normalization of the $(\nabla\varphi)^2$ term]. Therefore $\sigma\propto\mu b_z^2/a^2\propto\mu$ (see, e.g., Ref. [12]) which finally implies $B^{-1}\sigma/\lambda\approx 10^4$, supporting the statement below Eq. (10).

In conclusion, the above results show that the scenario of uniform motion of a straight dislocation line, coated by a new phase, does not apply in the regime $T_s(V)<T<T_0(V)$ where generically spinodal-like dynamic instabilities occur. The chances to observe these in experiments are especially promising for materials with a large striction effect at the transition. Candidates of such systems are in particular rare-earth metals for which the two-length-scale phenomenon has been observed [23], and recently related to the presence of dislocations [24].

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