Dislocation patterning in fatigued metals as a result of dynamical instabilities

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The nucleation of persistent slip bands in stressed materials is described as a cooperative phenomenon for dislocation populations. It is the competition between their mobility and their nonlinear interactions (creation, annihilation, and pinning) which causes the instability of uniform dislocation distributions versus inhomogeneous ones and leads to the formation and persistence of dislocation patterns.

INTRODUCTION

Current studies on fatigue failure in metals emphasize the role of persistent slip bands (PSBs) with their characteristic ladderlike structure in the initiation of cracks.[1,2] The ladderlike structure is composed by an alternate succession of rich and poor dislocation regions characterized by an intrinsic wavelength. These microstructural nonuniformities are a general feature of a large class of materials and although they may differ from one material to another with respect to structural details they always induce strain localization and act as preferential sites for microcrack nucleation.

In accordance with the observation that the development of PSBs in crystals under cyclic loading corresponds to a plateau in the stress-strain curve, a two-phase model has been developed which interprets this phenomenon as the result of a phase transitionlike behavior. The two phases are identified with the soft and hard material regions and this analogy has led to good qualitative agreement with experimental observations.[3,4] However, important questions related to the nucleation of PSBs within the surrounding vein structure of the matrix, the characteristic wavelength of the patterns, and their stability and relaxation when the stress is removed, have not been addressed and remain unanswered.

In an effort to elucidate these questions, we propose a reaction-diffusion scheme for the dynamics of the dislocation populations in fatigued metals able to reproduce the characteristics of the dislocation patterns for increasing stress amplitudes. Some ingredients of this model have already been discussed in previous communications,[5] where a detailed elaboration on one and two dimensional aspects was given.

DISLOCATION MICROSTRUCTURES

According to detailed experimental investigations mainly of copper single crystals, two types of dislocation patterns are formed in fatigued metals at low to intermediate stress amplitudes. One is the matrix or vein structure consisting of dense multipoles of primary edge dislocations (veins) separated by dislocation poor regions (channels). The width of both the veins and the channels is of the order of 1.2 μm, and the dislocation density is of the order of 10^{15} m^{-2} in the veins and $\simeq 6.5 \times 10^{11}$ m^{-2} in the channels. The second structure is ladderlike and corresponds to PSBs (see Fig. 1). It develops in primary slip planes and is formed by the successive alternation of dislocation poor regions ($\simeq 10^{13}$ m^{-2}) and of regularly spaced walls of high dislocation density ($\simeq 10^{15}$ m^{-2}). The wavelength of the pattern is distributed around a peak at 1.4 μm and its wave vector is parallel to the direction of the applied resolved shear stress.[6–10]

Moreover, the experimental data and simple theoretical models lead to a plateau in the cyclic stress-strain curve which corresponds to the formation of PSBs in the matrix and to the progressive filling of the sample with PSBs (see Fig. 2). The analogies with phase transitions which have been deduced from such curves[11,12] are an important step in the understanding of this phenomenon but are too superficial to render all of its richness mainly because it is related to the nucleation of a highly anisotropic structure in a nearly isotropic one.

The experimental observations also lead to the conclusion that the dislocation patterns within the PSBs are the

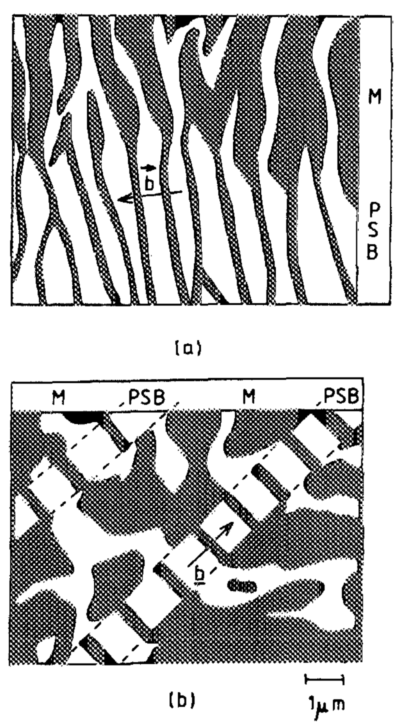

FIG. 1. Dislocation patterns showing matrix and PSB structures in slip (a) and cross-slip (b) planes. High dislocation density domains correspond to dark regions.[9–10]

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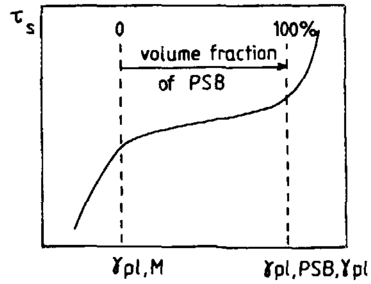

FIG. 2. Typical stress-strain curve for copper monocrystals under cyclic loading.

result of a dynamic equilibrium between different processes such as creation, annihilation, pinning, and diffusion. This is reminiscent of self-organization phenomena in other driven systems,[13,14] where the competition between nonlinearities and diffusivities lead to instabilities which induce different kinds of spatial patterns (e.g., Rayleigh–Bénard, Taylor–Couette, Turing instabilities). It appears, therefore, that reaction-diffusion equations could be appropriate to describe the dislocation dynamics, their motions, and interactions. This justifies our attempt to build a minimal model for the spatial ordering of dislocation populations based on balance equations deduced from a few, now well-established assumptions.

REACTION-DIFFUSION MODEL

We consider the creation of dislocations under an applied external stress by means of internal sources such as Frank–Read and Bardeen–Herring sources. Accordingly, the dislocation population is sufficiently high to be represented by a continuous dislocation concentration on a space scale larger than a few lattice spacings. Moreover, creation mechanisms compete with dynamical annihilation processes during glide which are operative even at low temperatures.

Furthermore, when the applied shear stress reaches a sufficiently high value or when thermal activation dominates local energy barriers, dislocations may break free and move rapidly with a stress-dependent velocity.[15] Hence, the dislocation populations may be divided in slow (gliding, climbing, cross-slipping, or even pinned at obstacles) and fast (freed by high shear stresses) ones. Such a distinction has also been made earlier[5,15] with the names immobile and mobile assigned, respectively, to the slow and fast moving dislocations.

The local concentrations of these two dislocation populations ρ_S and ρ_F are assumed to obey the following balance equations:

$$\left.\begin{aligned} \dot{\rho}_S + \operatorname{div} \mathbf{j}_S &= a - b\rho_S^2 - c\rho_S^3 - \beta\rho_S + \gamma\rho_F\rho_S^2, \\ \dot{\rho}_F + \operatorname{div} \mathbf{j}_F &= \beta\rho_S - \gamma\rho_F\rho_S^2, \end{aligned}\right\} \quad (1)$$

where a, b, c represent creation and annihilation rates of slow dislocations; $\beta\rho_S$ gives the rate of production of fast dislocations liberated by the applied stress when it surpasses a threshold value; and γ corresponds to the pinning rate of fast moving dislocations by practically immobile dipoles.

The coefficient β becomes operative above a certain threshold stress and it may generally depend on various mechanical fields such as the stress, strain, and their rates. For instance, in certain circumstances, β may be taken to vary linearly with the local rate of plastic deformation $\dot{\epsilon}$ which, in turn, may be written as $\dot{\epsilon} = \dot{\epsilon}_0 \exp\left[(A/T)(\tau - \tau_0 - B\sqrt{\rho_S})\right]$ where τ is the applied stress with τ_0 being its threshold value, and $B\sqrt{\rho_S}$ is the back stress due to slow dislocations. The various rate constants are directly related to the shear modulus and the Burgers vector and they may also depend on the temperature T, impurity density, as well as stacking fault energy. In a simpler situation, β may be proportional to $h(\tau - \tau_0)\tau^m$, where h is the usual Heaviside function and m a growth coefficient.

The next step is to develop an expression for the currents $\mathbf{j}_S$ and $\mathbf{j}_F$. While a mechanical procedure[15,16] is possible, leading to appropriate expressions of diffusive type for the dislocation fluxes, we adopt here a somewhat different approach based on the introduction of chemical-like potentials for the dislocation species. Indeed, this assumption of the existence of potentials is the only one reminiscent of an underlying possible thermodynamics structure. Other thermodynamic questions such as the correct form of the energy equation and the appropriate form of a dissipation inequality for dislocation species are rather involved and delicate subjects and are not addressed in this presentation. Under these circumstances, we can write the flux $\mathbf{j}_S$ as

$$\mathbf{j}_S = -\mathbf{M}_S \nabla \mu_S, \quad (2)$$

where $\mathbf{M}_S$ is the mobility tensor and μ_S the chemical potential-like variable.

In the framework of a statistical mechanical analysis based on the elasticity energy, μ_S may be written as

$$\mu_S(\mathbf{r}) = E_c + \int d\mathbf{r}' J(|\mathbf{r} - \mathbf{r}'|) f(\mathbf{r}') \rho(\mathbf{r}'), \quad (3)$$

where E_c is the core energy of dislocations, J the pair interaction, and f is a distribution function taking into account the possibility for the Burgers vector to be positive or negative. Due to the screening effect of dislocations of different Burgers vectors, the pair interaction is effectively short ranged and $\mu_S(\mathbf{r})$ may be approximated by the expression (a similar approximation was adopted in another paper[17])

$$\mu_S(\mathbf{r}) \simeq E_c + J^{(0)}\rho_S(\mathbf{r}) + J_{ij}^{(1)} \nabla_i \nabla_j \rho_S(\mathbf{r}), \quad (4)$$

where $J^{(0)} = \int d\mathbf{r} J(\mathbf{r}) f(\mathbf{r})$ and $J_{ij}^{(1)} = \frac{1}{2}\int d\mathbf{r}\, r_i r_j J(\mathbf{r}) f(\mathbf{r})$. Hence, we have

$$j_{S,i} = M_{ij} \nabla_j (J^{(0)}\rho_S + J_{kl}^{(1)} \nabla_k \nabla_l \rho_S), \quad (5)$$

where M_{ij} and $J_{kl}^{(1)}$ take into account the lattice structure and the orientations of slip and cross-slip planes. For the sake of simplicity in the qualitative discussion we pursue here, the mobility tensor will be considered as diagonal. Moreover, we will assume that the mobilities associated with slipping and climbing/cross slipping are such that $M_{xx} \simeq M_{yy} \gg M_{zz}$. The coordinate x denotes the slip direction, z the direction perpendicular to it on the slip plane, while the coordinate y being normal to the slip plane measures the effective mobility due to climbing the cross slipping effects. In the notation of Part III of a related paper[5] the axes y and z were interchanged for convenience.

As the shear stress points in the x direction, the dominant part of the current associated with the mobile dislocations should be proportional to their glide speed v. Various empirical relationships between v and the stress intensity have been proposed ranging from a power law $v = v_0(\tau/\tau_0)^m$ to exponential expressions of the type $v = v_0 \exp[-(\tau_0/\tau)^m]$. They only emphasize the fact[18,19] that v is negligible below the threshold stress τ_0 and jumps to a finite value beyond threshold. Moreover, as the applied stress (and hence the velocity) is periodically reversed in cyclic experiments that we are concerned with here, the effective current is diffusive on time scales longer than the period of the cyclic loading. This, together with the fact that positive and negative dislocations move in opposite directions at each stress reversal, leads rigorously to the following expression for the flux j_F

$$j_F = -D\nabla_x \rho_F, \tag{6}$$

with D being of the order of the thermal diffusivity below τ_0 and increasing rapidly to its maximum value above τ_0.

INSTABILITIES AND PATTERNS

The model proposed in the preceding section is inhomogeneous and contains nonlinear couplings between different variables. Hence, exact solutions are, in general, difficult to obtain. However, as we are interested in the evolution of the dislocation populations to their steady states, the problem may be simplified by the use of the slow mode dynamics which is able to describe the asymptotic dynamics of the system with a reduced number of spatially inhomogeneous variables. Effectively, the slow or unstable modes which play here the role of "an order parameter" are just the eigenmodes associated to the eigenvalues of the linear evolution matrix corresponding to the longer time scales of the problem. The fast modes may usually be adiabatically eliminated according to the so-called "slaving principle" leading to the reduction of the full nonlinear problem to its dominant aspects in the long time limit.[20]

The slow mode σ may be expressed here as a linear combination of the deviations from the homogeneous steady-state concentrations ρ_S^0 and $\rho_F^0[g(\rho_S^0) \equiv a - b\rho_S^{02} - c\rho_S^{03} = 0$, $\rho_F^0\rho_S^0 = \beta/\gamma$, and its Fourier transform σ_q is found to obey the following kinetic equations

$$\dot{\sigma}_{\mathbf{q}} = \omega_{\mathbf{q}}\sigma_{\mathbf{q}} - v\int d\mathbf{k}\,\sigma_{\mathbf{q}-\mathbf{k}}\sigma_{\mathbf{k}} - u\int d\mathbf{k}\int d\mathbf{k}'\sigma_{\mathbf{q}-\mathbf{k}-\mathbf{k}'}\sigma_{\mathbf{k}}\sigma_{\mathbf{k}'}, \tag{7}$$

where

$$\omega_q = \tfrac{1}{2}\{\omega_1 - \omega_2 + [(\omega_1 + \omega_2)^2 - 4\beta\gamma\rho_S^{02}]^{1/2}\}, \tag{8}$$

and

$$\left.\begin{aligned} \omega_1 &= r + \beta - d_\parallel(q_x^2 + q_y^2 - q_0^2)^2 - d_\perp q_z^2, \\ \omega_2 &= \gamma\rho_S^{02} + q_x^2 D, \end{aligned}\right\} \tag{9}$$

with

$$\left.\begin{aligned} r &= M_{xx}\frac{|J^{(0)2}|}{4|J^{(1)}|} + g'(\rho_S^0), & q_0^2 &= \frac{|J^{(0)}|}{2|J^{(1)}|}, \\ d_\parallel &= M_{xx}|J^{(1)}|, & d_\perp &= (M_{xx} - M_{zz})\frac{|J^{(0)}|}{2}. \end{aligned}\right\} \tag{10}$$

The quantities u and v are algebraic functions of the various constants appearing in (1) with u being positive. Also, we have assumed that $J_{kl}^{(1)}$ in Eq. (5) is isotropic, i.e. $J_{kl}^{(1)} = J^{(1)}S_{kl}$.

Hence, below and not too far above threshold, ω_q may be safely approximated to be

$$\omega_q = r - d_\parallel(q_x^2 + q_y^2 - q_0^2)^2 - d_\perp q_z^2 + \beta\frac{q_x^2}{q_x^2 + q_1^2}, \tag{11}$$

with

$$q_1^2 = \frac{\gamma\rho_S^{02}}{D}. \tag{12}$$

This approximation fails far above threshold where the slow mode dynamics may even include oscillations.[5] Such effects will, however, not be considered in the present analysis.

According to the enhancement of the dislocation mobility and of the creation rate of free dislocations, different regimes and steady states may be obtained from the slow mode kinetics (11) for increasing stress intensity. For convenience, we discuss these possibilities in four distinct stages as follows:

(1) At low values of stress, mobilities and plastic deformation rates are vanishingly small ($r < 0, \beta \simeq 0$). Consequently, the homogeneous dislocation density $\rho_S = \rho_S^0$, $\rho_F^0 = 0$ is stable.

(2) For higher values of stress but still below the threshold τ_0, the mobility increases while β remains negligible. Hence, r may become positive leading to the instability of the homogeneous density versus inhomogeneous perturbations. In the idealized case discussed here ($M_{xx} \simeq M_{yy} \neq M_{zz}$), the fastest growing fluctuations correspond to wave vectors q such that $q_x^2 + q_y^2 = q_0^2$ and $q_z = 0$ and the steady dislocation structure which is the most likely to appear corresponds to maximum of the dislocation density distributed on rodlike patterns of triangular symmetry which may be associated with the vein structure of the matrix (see Fig. 3). It is noted that a set of wave vectors defined by $r - d_\parallel(q_x^2 + q_y^2 - q_0^2)^2 - d_\perp q_z^2 > 0$ are allowed for this structure. Moreover, as the pattern appears via the spontaneous breaking of continuous symmetries it is expected to be extremely sensitive to even small inhomogeneities. Hence, the real structures are presumably less regular than the ones predicted by the fastest growing fluctuation argument in agreement with experimental observations.[21]

(3) When the stress reaches the threshold $\tau = \tau_0$, inho-

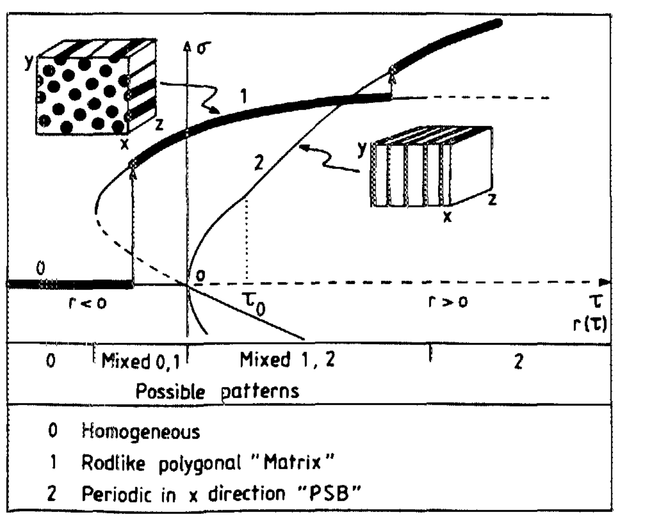

FIG. 3. Schematic bifurcation diagram for Eq. (7): σ is the amplitude of the spatial patterns with wave number q_0. Plain lines represent stable states, dashed lines unstable ones, and heavy lines give the preferred states (minimizing the Lyapunov functional).

mogeneous fluctuations with wave vectors in the x direction become favored as the result of the anisotropy induced by the breaking free of dislocations in this direction. Hence, a competition may occur between the now deformed polygonal rodlike structures associated with the veins and the layer ladderlike periodic structures in the x direction corresponding to PSBs. It turns out that the preferred wave number q_c of this pattern is given by the relation

$$2d_{\parallel}(q_c^2 - q_0^2) - \beta \frac{q_1^2}{(q_c^2 + q_1^2)^2} = 0, \tag{13}$$

and is hence slightly larger than q_0.

(4) If the stress is increased further, a new threshold appears beyond which the rodlike structures become definitely unstable versus the ladderlike pattern which then completely fills the system.

CONCLUSIONS AND PERSPECTIVES

By the association of the vein and PSBs structures with the rodlike polygonal and ladderlike layered patterns described in the previous section various experimental observations are qualitatively recovered.[9,10,22] Effectively, beyond threshold, matrix and PSBs are metastable and as a result of their competition PSBs may nucleate within the vein structure. Moreover, the increase of the local plastic deformation rate corresponds to higher anisotropy and induces a continuous deformation of the matrix structure. When the matrix becomes unable to accommodate such changes it turns unstable and the ladderlike structure may fill the entire system.

Due to the continuous symmetry breaking, phase fluctuations may be important. For example, a complete shift of the structure as a whole should be very easy. A shift of the ladder walls by the gliding of the pattern in the cross-slip plane has actually been observed.[10] Furthermore, stable patterns with different wave vectors are possible, but their wavelengths are distributed around the value corresponding to the fastest growing fluctuations, in accordance with experimenal observations. Moreover, stationary phase fluctuations of the patterns may also exist leading eventually to layer splitting of the wall structure, this effect being also observed experimentally.

To conclude, let us emphasize the fact that the model presented here provides a conceptual framework dedicated to the study of the formation of dislocation patterns as a result of a competition between nonlinear interactions and stress enhanced mobility. The main features of pattern formation, pattern selection, and sensitivity observed in other nonequilibrium driven systems are recovered. However, the qualitative agreement with experimental findings needs further confirmation and the predictive power of the model needs to be tested with realistic numerical values of the rate and diffusion constants. In this connection, numerical simulations based on the system (1) and dedicated to the dynamical aspects of the nucleation process of PSBs from the matrix will be performed in future works.

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