Solitary charge-density wave in an ensemble of dislocations

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The nonlinear dynamics of perturbations of the dislocation density and of the dislocation charge density is analyzed on the basis of a system of evolution equations. A solitary wave exists in an ensemble of dislocations. It takes the form of a jump for the total dislocation density and the form of a soliton for the excess density. The stability of the self-similar solutions found is analyzed. There is a region of parameter values in which steady-state wave solutions are stable. The spectrum of possible values of the propagation velocity of a solitary wave is found. © *1995 American Institute of Physics.*

1. INTRODUCTION

Describing the evolution of the microstructure of a material during loading and its relationship with the rheology of plastic flow is a central problem in the physical theory of strength and plasticity. A basic goal of the theory is to explain the complex onset and development of dislocation structures during plastic deformation of a material observed experimentally. Although progress has been made in experimental research on deformable solids, we do not yet have a generally accepted picture or, especially, a rigorous quantitative theory for describing these phenomena. In particular, much is still unclear regarding the mechanisms for the formation of glide bands, localized-shear bands, Lüders' bands, dynamic dislocation formations of a common sign, etc.[1–4] On the other hand, enough information has been gathered that it is possible to interpret the processes of plastic deformation from a common standpoint: the nonlinear dynamics of a deformable crystal.[3] Mathematically, the problem of studying these processes theoretically can be formulated on the basis of a system of nonlinear evolution equations for the density of continuously distributed dislocations. The evolution equations are a consequence of the fundamental law that the Burgers vector of a system of dislocations is conserved. This consequence of the law remains in force in the course of dislocation multiplication and various dislocation reactions.[5,6]

In this letter we examine in detail the dynamics of an ensemble of dislocations for the case of one glide system. We incorporate the generation, recombination, and sinking of dislocations with the goal of finding self-similar solutions in the form of solitary waves of the dislocation density.

2. EVOLUTION EQUATIONS

The differential form of the conservation law for the Burgers vector in a crystal is the compatibility equation $\partial\alpha_{ik}/\partial t + e_{iem}\partial j_{mk}/\partial x_l = 0$, which relates the dislocation density tensor

$$\alpha_{ik} = \sum_s \tau_i b_k^s \rho_s$$

and the dislocation flux tensor[6]

$$j_{ik} = e_{ijm}\sum_s \tau_j b_k^s \rho_s V_m^s .$$

The tensors α_{ik} and j_{ik} are expressed in terms of the scalar dislocation density $\rho_s(\mathbf{r},t,\boldsymbol{\tau})$. For this purpose, one can derive a system of evolution equations from the compatibility equation, allowing for local interactions of dislocations:[5,7]

$$\frac{\partial \rho_s}{\partial t} + \mathrm{div}\rho_s \mathbf{V}^s = F_s(\rho_1, \rho_2 ...). \tag{1}$$

Here $\mathbf{V}^2$ is the average glide velocity of the dislocations, $\boldsymbol{\tau}$ is the unit vector tangent to the dislocation line, and the subscript s is a number which specifies a possible direction of the Burgers vector $\mathbf{b}$ of the dislocation. The nonlinear functions $F_s(\rho_1, \rho_2 ...)$ describe the change in the density of dislocations in the course of their interaction. These functions satisfy the condition $\Sigma_s \tau_i b_k^s F_s = 0$, which expresses the fact that the Burgers vector is conserved in these processes.

Inertial effects are negligible in essentially all methods for deforming a crystal, except shock loading. The motion of the dislocations can thus be assumed to be quasisteady.[5] In this case the average dislocation velocity V^s can be expressed algebraically in terms of the external stress field σ^e and the internal stress field $\sigma^i(\mathbf{r},t)$ (Refs. 2 and 5). In the initial stage of the deformation of the material, the relation $\sigma^i \ll \sigma^e$ holds, and the dislocation velocity $V^s \simeq V^s(\sigma^e)$ can be assumed to remain constant.[4,5] We restrict the analysis of the present letter to this case.

We consider a deformable crystal which is oriented for single glide. In this case the plastic-deformation process develops along a given glide system. We accordingly assume that dislocations of a common type ($\boldsymbol{\tau} \| \mathbf{b}$), characterized by densities $\rho_+(x,t)$ and $\rho_-(x,t)$ (and by respective "charges" b and $-b$), participate in the evolution of the ensemble of dislocations. These dislocations are assumed to be moving opposite each other along the x direction in parallel glide planes, at constant velocities $V_+ = V$ and $V_- = -V$, to be multiplying by the mechanism of double transverse glide, and to be participating in annihilation and sinking processes. Taking these processes into account, we can write the system of evolution equations in (1) in the form

$$\frac{\partial \rho_\pm}{\partial t} + \frac{\partial}{\partial x}(\rho_\pm V_\pm) = A(\rho_+ + \rho_-) - c\rho_\pm - \kappa\rho_+\rho_- . \tag{2}$$

Here A is the coefficient of dislocation multiplication in accordance with the mechanism of double transverse glide, $\kappa \simeq 2hV$ is an annihilation coefficient (h is the radius of the trapping of dislocations into dipole configurations), and $c \simeq hV\rho_c$ is a dislocation sinking coefficient (if the obstacles are primarily of a dislocation nature, ρ_c is the density of immobile dislocation complexes).

System (2) has two equilibrium states: $\rho_+ = \rho_- = 0$ and $\rho_+ = \rho_- = (4A - c)/\kappa = \beta/\kappa = \rho_0/2$. We introduce the dimensionless variables $n = (\rho_+ + \rho_-)/\rho_0$ and $m = (\rho_+ - \rho_-)/\rho_0$, which characterize the total dislocation density and the dislocation charge, respectively. In dimensionless variables, Eqs. (2) become

$$\frac{\partial n}{\partial t} + V\frac{\partial m}{\partial x} = \beta n(1-n) + \beta m^2,$$

$$\frac{\partial m}{\partial t} + V\frac{\partial n}{\partial x} = -cm. \tag{3}$$

3. STEADY-STATE SOLITARY WAVES

For system (3) we assume that the functions $n(x,t)$ and $m(x,t)$ satisfy the boundary conditions $n(-\infty,0) = m(\pm\infty,0) = 0$, $n(\infty,0) = 1$. These conditions actually correspond to the beginning of dislocation multiplication at the right side of the sample.

We seek solutions of system (3) in the class of self-similar solutions, assuming $m = m(x+ut)$, $n = n(x+ut)$. Substituting a solution of the assumed form into the original system of equations, (3), we find a system of equations for the self-similar variable $\xi = x + ut$:

$$(1-\gamma^2)\frac{dn}{d\xi} = -\beta[\gamma n(1-n) + \alpha m + \gamma m^2],$$

$$(1-\gamma^2)\frac{dm}{d\xi} = \beta[n(1-n) + \alpha\gamma m + m^2] \tag{4}$$

with the boundary conditions $n(-\infty) = m(\pm\infty) = 0$, $n(\infty) = 1$. Here we have introduced the dimensionless parameters $\gamma = uV$, $\alpha = c/\beta$. System (4) has two fixed points, (0, 0) and (1, 0), in the (n,m) plane. Linearizing system (4) near the (0, 0) state, and making the substitutions $n,m \sim \exp(\mu\beta\xi)$, we find a characteristic equation, from which we in turn find

$$\mu_{1,2} = \frac{\gamma(\alpha-1) \pm \sqrt{\gamma^2(\alpha-1)^2 - 4\alpha(1-\gamma^2)}}{2(1-\gamma^2)}. \tag{5}$$

Since the density $n(x,t)$ cannot be negative, we have $\gamma^2(\alpha-1)^2 - 4\alpha(1-\gamma^2) \geqslant 0$. Hence

$$\gamma \geqslant \gamma_{\min} = 2\frac{\sqrt{\alpha}}{1+\alpha}. \tag{6}$$

It follows from (5) that for values $\gamma_{\min} \leqslant \gamma < 1$ the (0, 0) state is a node; if $\alpha > 1$, it is unstable, while if $\alpha < 1$, it is stable. It is not difficult to show that the second singular point, (1, 0), is a saddle point under the condition $\gamma^2 < 1$. Only two trajectories pass through this saddle point. Working from these results, we can draw a phase diagram near

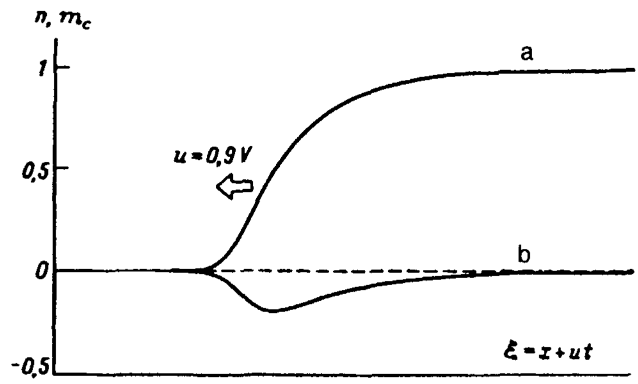

FIG. 1. Solitary wave of the total dislocation density (a) and of the dislocation charge density (b) corresponding to a self-similar solution of system of equations (4) for the parameter values $\alpha=2.5$ and $\gamma=\gamma_{\min}(\alpha)=0.9$.

the singular points, and we can draw a trajectory of a wave solution of system (4), which runs from the unstable node (0, 0) to the saddle point (1, 0). Corresponding to this trajectory are solutions in the form of a traveling jump for $n(\xi)$ and a pulse for $m(\xi)$, as shown in Fig. 1. It follows from an analysis of the steady-state solutions of system (4) that solitary waves can propagate under the condition $\alpha>1$ at a velocity $u\in[u_{\min},V]$, where $u_{\min}=2V\sqrt{\alpha}/(1+\alpha)$.

Let us consider the limit $\alpha\gg 1$. If the sinks are of a dislocation nature, then it is not difficult to see that we have $\alpha=\rho_c/\rho_0$. In other words, this case corresponds physically to an intense immobilization of dislocations. System (3) reduces in this case to an equation for $n(x,t)$:

$$\frac{\partial n}{\partial t}=\beta n(1-n)+D\frac{\partial^2 n}{\partial x^2},\quad D=\frac{V^2}{c}. \tag{7}$$

This equation, known as the Fischer equation, was first studied in Refs. 8 and 9. Kolmogorov *et al.*[9] proved the existence of self-similar solutions of a traveling type, $n(\xi)=n(x+ut)$, with a spectrum of possible values of the velocity bounded from below ($u\geqslant u_{\min}=2\sqrt{D\beta}$). It is not difficult to see that under the condition $\alpha\gg 1$ the expression for the minimum possible propagation velocity of a solitary wave $u_{\min}=2V\sqrt{\alpha}/(1+\alpha)$, becomes the expression $u_{\min}=2V/\sqrt{\alpha}$, which was derived in Ref. 9 for the Fischer equation. A qualitatively new point for system (3), which distinguishes it from the Fischer equation, is that the spectrum of possible velocity values is a continuum, with not only a lower boundary but also an upper boundary, the dislocation velocity. Another qualitatively new point is that a solitary wavefront exists only if the density of sinks is sufficiently large ($\alpha>1$).

4. STABILITY OF SELF-SIMILAR SOLUTIONS

Let us examine the stability of steady-state solutions $n_c(\xi)$ and $m_c(\xi)$ with respect to the class of perturbations which are limited to a finite region, e.g., $[-L,L]$. For this purpose we seek a solution of the original system, (3), in the form

$$n(\xi,t)=n_c(\xi)+\delta n(\xi,t), \qquad \delta n(\xi,t)=n_p(\xi)e^{\lambda t},$$
$$m(\xi,t)=m_c(\xi)+\delta m(\xi,t), \quad \delta m(\xi,t)=m_p(\xi)e^{\lambda t}.$$

Assuming that the perturbations δn and δm are small, we find an eigenvalue problem for the eigenfunctions $n_p(\xi)$ and $m_p(\xi)$ and the eigenvalues λ:

$$\frac{d}{d\xi}(m_p+\gamma n_p)=n_p[1-\lambda-2n_c]+2m_p m_c,$$

$$\frac{d}{d\xi}(n_p+\gamma m_p)=-(\lambda+\alpha)m_p. \tag{8}$$

Here we have the boundary conditions $n_p(\pm L)=m_p(\pm L)=0$. Making the substitution

$$\psi(\xi)=(n_p+\gamma m_p)\exp\left\{\frac{1}{2}\int p(\xi)d\xi-\frac{\gamma\xi(\lambda+\alpha)}{1-\gamma^2}\right\},$$

where $p(\xi)=[\gamma(1+\alpha)-2(m_c+\gamma n_c)]/(1-\gamma^2)$, we can reduce system (8) to an equation which is self-adjoint in form:

$$\frac{d^2\psi}{d\xi^2}+[H(\lambda,\xi)-U(\xi)]\psi=0, \quad \psi(\pm L)=0, \tag{9}$$

where

$$H(\lambda,\xi)=-[\lambda^2+\lambda B(\xi)]/(1-\gamma^2)^2,$$

$$B(\xi)=\alpha-1+2n_c(\xi)+2\gamma m_c(\xi),$$

$$U(\xi)=[\gamma^2(1+\alpha)/4-\alpha+q(\xi)]/(1-\gamma^2)^2,$$

$$q(\xi)=\gamma(\alpha-1)(m_c+\gamma n_c)+(2\alpha-1)(1-\gamma^2)n_c+(n_c+\gamma m_c)^2. \tag{10}$$

A study of the spectral properties of problem (9), in which the quantity H is quadratic in λ (in contrast with the situation in the steady-state Schrödinger equation), is a problem in the theory of self-adjoint quadratic beams.[10,11] It follows from this theory[10] that in the case $B,U\geq 0$ the spectrum of characteristic numbers of the beam, $L(\lambda)=-d^2/d\xi^2-H+U$, lies in the left half-plane; i.e., we have $\mathrm{Re}\lambda\leq 0$. The value at $\lambda=0$ is not an eigenvalue of problem (9), since the perturbations $\delta n(\xi)=dn_c/d\xi$ and $\delta m(\xi)=dm_c/d\xi$ corresponding to this value are defined on the entire real axis and thus do not satisfy the boundary condition $\delta m(\pm L)=\delta n(\pm L)=0$. This statement means that under the conditions $B,U\geq 0$ the perturbations $\delta n(\xi,t)$ and $\delta m(\xi,t)$ are damped exponentially in time, and self-similar, steady-state solutions are asymptotically stable. Analysis of the operators B and U in (10) shows that the conditions $B,U\geq 0$ hold under the conditions

$$\alpha>1, \quad \gamma_{\min}(\alpha)\leq\gamma<1, \tag{11}$$

where $\gamma_{\min}$ is given by expression (6).

5. DISCUSSION OF RESULTS

This analysis thus shows that system (3) with the initial conditions $n(x,0)=n_c(x,\gamma)$ and $m(x,0)=m_c(x,\gamma)$ ($\gamma \in [\gamma_{\min},1]$, $x \in R$) has a self-similar solution of the traveling-wave type with a velocity $u=\gamma V$. This solution is stable with respect to the class of perturbations which are confined to a finite region. In examining the stability of steady-state solutions with respect to perturbations which are given on an infinite interval, it becomes necessary to incorporate neutral models of the shear type, which usually violate the asymptotic stability of steady-state wave solutions in problem of this sort.[12,13] Under more natural, finite initial conditions, where there is no problem of neutral solutions, there is the important question of estimating the steady-state wave propagation velocity. This problem has been discussed in the literature[9,14-16] for nonlinear equations of the parabolic type $y_t-y_{xx}=f(y)$ ($y \in [0, 1]$, $f(0)=f(1)=0$). It has been established that for convex functions $f(y)$ a transition from unstable to stable steady states occurs after a long time, by means of switching waves, whose velocity is determined unambiguously by the linear part of the corresponding equation.[15,16] It was shown in Ref. 17 that corresponding results are valid for a broader class of problems, in particular, systems of a hyperbolic type.

Following Ref. 17, we linearize expressions (3). For the variable $m(x,t)$ [or for $n(x,t)$] we then find the equation

$$m_{tt}-V^2m_{xx}+2\sqrt{c\beta}\delta m_t=c\beta m, \quad \delta=\frac{\alpha-1}{2\sqrt{\alpha}}, \tag{12}$$

which has the same structure as the linearized sine-Gordon equation discussed in Ref. 17. It is thus possible to apply the result there to the case at hand. From the solution of Eq. (12),

$$m(x,t)\sim t^{-1/2}\exp\left\{\frac{\sqrt{c\beta}}{V}\left(x+\frac{Vt}{\sqrt{1+\delta^2}}\right)\right\},$$

we find an asymptotic estimate of the wave velocity:

$$u=\left|\frac{dx}{dt}\right|\simeq 2V\frac{\sqrt{\alpha}}{1+\alpha}-\frac{V}{2\sqrt{c\beta\cdot t}}.$$

It can be concluded that for system (3), under the condition $\alpha>1$, initial distributions $m(x,0)$ and $n(x,0)$ which are concentrated on a finite interval develop into traveling self-similar solutions $n_c(x+ut)$ and $m_c(x+ut)$ with a velocity $u=u_{\min}=2V\sqrt{\alpha}/(1+\alpha)$.

Let us look at some physical applications of this model. It follows from the results of this letter that, if the sink density ρ_c at the beginning of the multiplication of dislocations is greater than the initial density of mobile dislocations, ρ_0, then regions of elevated density of dislocations and dislocation charge can propagate in the form of solitary waves (Fig. 1) at a velocity $u\simeq 2V\sqrt{\alpha}/(1+\alpha)$. In the case $\rho_c<\rho_0$ ($\alpha<1$), steady-state waves cannot propagate, and a solution of the original system of equations should be sought in the class of time-varying solutions. This case was studied in Ref. 18 under the condition

$\alpha=0$. An evolution equation for the excess dislocation density (for the dislocation charge) was found from the original system of equations. Under certain assumptions that evolution equation reduces to a nonlinear Burgers equation. It was shown for an initial-value problem that, in cases in which effective conditions for the formation of dislocation pile-ups of a common sign arise, their subsequent separation and propagation take the form of a slowly damped shock front, specifically, a triangular wave. Accordingly, within the framework of this model, the primary type of dislocation structure in the initial stage of the deformation of the material, in which the density of sinks is small, is a pile-up of dislocations. As the density of sinks increases, and the critical value $\rho_c=\rho_0$ is reached, the formation of a new type of substructure becomes possible: a dislocation band (a region of elevated total dislocation density). The development of this band is accompanied by the propagation of a solitary wave of dislocation charge density. This conclusion confirms the experimental results of Ref. 19, according to which the nucleation of glide bands is preceded by a structure in the form of separate dislocation pile-ups, which formed in the initial stage of deformation.

We should bear in mind that since glide bands are generally 2D formations, a rigorous description of the growth dynamics and the shape of a glide band should be attainable in a systematic 2D formulation of the problem. That topic lies outside the scope of the present letter; a corresponding study will be published separately.

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[1] V. I. Al'shits and G. V. Berezhkova, *Physical Crystallography* [in Russian] (Nauka, Moscow, 1992).
[2] V. I. Vladimirov, *Physical Theory of Plasticity and Strength* [in Russian] (Izd. LPI, Leningrad, 1973).
[3] *Cooperative Deformation Processes and Localization of Strain* [in Russian] (Nauk. Dumka, Kiev, 1989).
[4] V. V. Rybin, Izv. Vyssh. Uchebn. Zaved., Fiz. **34**(3), 7 (1991).
[5] A. M. Kosevich, *Dislocations in Elastic Theory* [in Russian] (Nauk. Dumka, Kiev, 1978).
[6] L. D. Landau and E. M. Lifshitz, *Theory of Elasticity* [in Russian] (Nauka, Moscow, 1987).
[7] Sh. Ch. Khannanov, Fiz. Met. Metalloved. **46**, 708 (1978).
[8] R. A. Fischer, Ann. Eugenics, No. 7, 355 (1937).
[9] A. N. Kolmogorov, I. G. Petrovskiĭ, and N. S. Piskunov, Byull. MGU, Ser. A, Mat. Mekh. **1**, 1 (1937).
[10] M. G. Kreĭn and G. K. Langer, Dokl. Akad. Nauk SSSR **154**, 1258 (1964) [*sic*].
[11] I. Ts. Gokhberg and M. G. Kreĭn, *Introduction to the Theory of Linear Non-Self-Adjoint Operators* [in Russian] (Nauka, Moscow, 1965).
[12] J. Canosa, IBM J. Res. Dev. **17**, 307 (1973).
[13] D. H. Sttinger, Adv. Math. **22**, 312 (1976).
[14] D. G. Aronson and H. F. Weinberger, Adv. Math **30**, 33 (1978).
[15] W. van Saarlos, Phys. Rev. A **37**, 211 (1988); A **39**, 6367 (1989).
[16] M. Bramson, Met. Am. Math. Soc. **285**, 1 (1983).
[17] V. G. Kamenskiĭ and S. V. Manakov, JETP Lett. **45**, 638 (1987).
[18] O. V. Mareeva, G. F. Sarafanov, and S. N. Nagornykh, Fiz. Met. Metalloved. **75**, 37 (1993).
[19] C. Laird, P. Charsley, and H. Mugrabi, Mater. Sci. Eng. **81**, 433 (1986).

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