NANOSCALE STRAIN LOCALIZATION:
THE INSTABILITY OF STRAINIONS

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ABSTRACT

A new model of strain localization and damage band formation, inspired by population dynamics, is introduced in this paper. The basic assumption is that strain at nanoscales can be described by means of a kinetic model of molecular interaction. The strain energy induced by external sources concentrates at a numerable set of mobile entities, hereby called *"strainions"*. Under normal conditions these strain energy accumulators are uniformly distributed within the body. If the energy level between some molecules increases too sharply, for instance due to increasing strains, the strainions begin to dissipate heat energy and strain localization may occur. By coupling the Fick's law for diffusion and a classical conservation law for heat production, the random motion of heat energy can be modelled. A number of physical parameters are introduced in the model. These are a proportionality constant k that measures the strength of heat attraction (called the *"thermotaxis"* coefficient), a *"motility"* constant c, and a diffusion constant D. A differential system of two nonlinear equations is obtained, which admits the uniform solution, corresponding to the equilibrium state. Then, we investigate, through the method of small perturbations, if a sudden small disturbance to the uniform state remains local and extinguishes, or propagates in space and time, leading to strain localization and damage. We found that strain localization occurs if the motility c of the strainions or the decay rate of the heat concentration are small or, inversely, if the rate of heat production or the thermotaxis coefficient k are large.

1 INTRODUCTION

Pattern formation in Nature is often the result of system instabilities. In this context, strain localization and damage in geomaterials are multiscale phenomena. At the macroscales, cohesive crack propagation is characterized by strain softening and energy dissipation. A plenty of models has been proposed to explain cohesive cracking at the meso-level (i.e., at the level of the grains), taking into account several effects like strain gradients [1], bridging and friction. At the nano-scale of observation, band formation is observed (Figure 1), whose fractal structure suggests the existence of self-organization [2].
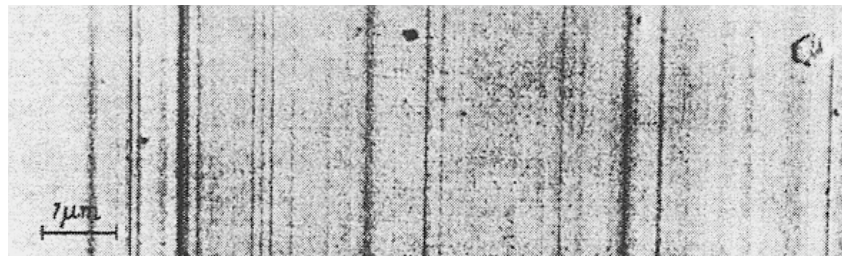

Figure 1. Slip lines in copper at the sub-micron scale (after Kleiser & Bocek, [3])

At nanoscales, surface effects are predominant, i.e. surface tension and friction affect the mechanical response [4]. Moreover, heat production occurs at the slip bands, and electromagnetic fields interact with the strain energy. There is a strong need to understand the mechanical properties of nanostructures. In particular, the mechanical stability of nanotubes and nanowires under severe stress-strain conditions needs to be assessed.

In this paper, a new model of strain localization and damage band formation is introduced. The theoretical framework is inspired by population dynamics [5]. The basic assumption is that strain at nanoscales can be described by means of a kinetic (diffusive) model of molecular interaction. Instead of the classical interatomic potentials field, we assume that the strain energy induced by external sources (loads, displacements or whatever) concentrates at a numerable set of mobile entities, hereby called *"strainions"*. Under normal conditions (e.g., if molecular spacing and thermal fluctuations do not exceed certain values), these strain energy accumulators are uniformly distributed within the body (Figure 2a). Continuous energy fluctuations at nanoscales cause a diffusion process: the strainions move away from regions of high strain concentration to regions of low strain concentration. Macroscopically, this equilibrium state corresponds to the homogeneous deformation of the continuum.

If the energy level between some molecules increases too sharply, for instance due to increasing strains, the strainions begin to dissipate heat energy. Such an heat source acts as an attractant for other strainions, due to the overall tendency to a minimum of the total energy of the system (what is usually called *stress redistribution* at macroscales). Therefore, strainions move toward the high concentrations of heat and tend to form aggregates (Figure 2b). These aggregates are called slip bands, i.e., regions of high strain localization and damage. By means of perturbation theory, it is possible to determine the conditions for such instability.

2. THE ONE-DIMENSIONAL KINETIC MODEL OF STRAINIONS

In order to formulate a simple model, we assume that changes take place only in one spatial dimension (z) and that all parameters are constant in any cross-section. Let $n(z,t)$ be the number of strainions per unit area at position z and at time t, and let $h(z,t)$ denote the concentration of heat production at (z,t). The time rate of change of the number of strainions in (z_1, z_2) must equal the number of strainions entering the region at $z=z_1$ minus the number of strainions leaving the region at $z=z_2$. If $\Psi(z, t)$ denotes the flux at z at time t, then the conservation law can be written as:

$$\frac{d}{dt}\int_{z_1}^{z_2} n(z,t)dz = \Psi(z_1,t) - \Psi(z_2,t) = -\int_{z_1}^{z_2} \frac{\partial}{\partial z}\Psi(z,t)dz .$$ (1)

If the functions are assumed to be smooth, the time derivative can be pulled inside the first integral. For an arbitrary interval of integration we get the differential form:

$$\frac{\partial n}{\partial t} + \frac{\partial \Psi}{\partial z} = 0$$ (2)

The constitutive form of the flux Ψ comes from the assumptions outlined in the introduction. Accordingly, Ψ is the sum of a flux Ψ_d due to random diffusion of the strainions and a flux Ψ_h due to attraction induced by heat production, that is: $\Psi = \Psi_d + \Psi_h$.

In the homogeneous condition, the strainions move from the regions of high concentration to those of low concentration of n, so that Ψ_d is proportional to the gradient of $n(z,t)$:

$$\Psi_d = -c\frac{\partial n}{\partial z}(z,t),\tag{3}$$

where $c>0$ is a constant of strainion motility. In the theory of diffusion, the above equation is named Fick's law. The expression for the other flux contribution can be easily determined if we state that Ψ_h is proportional to the gradient of heat production. Moreover, the heat being an extensive quantity, Ψ_h should also be proportional to the number n of strainions. Therefore we can write:

$$\Psi_h = kn(z,t)\frac{\partial h}{\partial z}(z,t),\tag{4}$$

where $k>0$ is a proportionality constant that measures the strength of heat attraction (call it a *"thermotaxis"* coefficient). Combining the two flux contributions we get the following nonlinear partial differential equation:

$$\frac{\partial n}{\partial t} = \frac{\partial}{\partial z}\left(c\frac{\partial n}{\partial z} - kn\frac{\partial h}{\partial z}\right).\tag{5}$$

Because there are two unknown functions (i.e. $n(z,t)$ and $h(z,t)$), another equation is still required. This is a conservation law for heat production:

$$\frac{\partial h}{\partial t} = -\frac{\partial \varphi_h}{\partial z} + H,\tag{6}$$

where $\varphi(z, t)$ represents the heat flux via diffusion and $H(z, t)$ denotes the amount of heat generated at time t per unit volume.

The random motion of heat energy can be modelled, similarly to the previous assumptions, by means of a proportionality of flux to the gradient, through a diffusion constant D, i.e.:

$$\varphi_h = -D\frac{\partial h}{\partial z},\tag{7}$$

whereas the source term H can be conveniently written as:

$$H = q_1 n - q_2 h,\tag{8}$$

where q_1 is the rate of heat production of the strainions and q_2 is the rate of heat diffusion outside the body. The second equation of the problem is therefore obtained as:

$$\frac{\partial h}{\partial t} = D\frac{\partial^2 h}{\partial z^2} + q_1 n - q_2 h.\tag{9}$$

The differential system formed by eqs. (5) and (9) has the uniform solution: $n(z,t) = n_0$ and $h(z,t)=h_0$ - where n_0 and h_0 are constants - provided that $q_1 n_0 = q_2 h_0$. The uniform state (Figure 2a) is therefore an equilibrium solution.
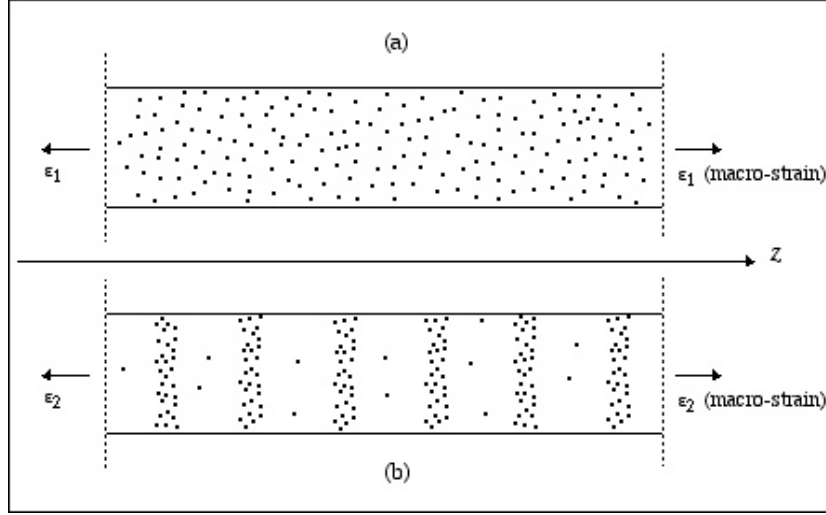

Figure 2. Uniformly distributed strainions (a) and onset of slip band formation (b).

3. ONSET OF STRAIN LOCALIZATION AS AN INSTABILITY OF THE UNIFORM STATE

We investigate now, through the method of small perturbations, if a sudden small disturbance to the uniform state remains local and extinguishes, or propagates in space and time, leading to strain localization and damage. If n^* and h^* are small departures from the equilibrium state, we can put the quantities $n(z,t)= n_0 + n^*(z,t)$ and $h(z,t)=h_0 + h^*(z,t)$ into the differential system, obtaining:

$$n_t^* = \frac{\partial}{\partial z}\left(cn_z^* - kn_0 h_z^* - kn^* h_z^*\right), \tag{10-a}$$

$$h_t^* = Dh_{zz}^* + q_1 n^* - q_2 h^*. \tag{10-b}$$

Since the quadratic term $n^* h_z^*$ is smaller than the linear terms, eq. (10-a) can be linearized into:

$$n_t^* = cn_{zz}^* - kn_0 h_{zz}^* \tag{11}$$

which is the companion to eq. (10-b). The coupled partial differential equations are diffusion-like and therefore admit a solution in the form of a Fourier mode:

$$n^* = C_1 e^{\alpha t} e^{i\beta z}, \tag{12-a}$$
$$h^* = C_2 e^{\alpha t} e^{i\beta z}, \tag{12-b}$$

where C_1, C_2, α and β are constants. If $\alpha>0$ the Fourier mode for the perturbation would grow in time and thus the uniform state would be unstable to small perturbations. In order to check the existence of solutions like eqs. (12) we insert them in the differential system, obtaining a homogeneous system of algebraic equations for C_1 and C_2:

$$\left(\alpha + c\beta^2\right)C_1 - kn_0\beta^2 C_2 = 0, \tag{13-a}$$

$$-q_1 C_1 + \left(\alpha + D\beta^2 + q_2\right)C_2 = 0. \tag{13-b}$$

Nontrivial solutions require that the determinant of the coefficient matrix vanishes. This yields a quadratic equation with two real roots in α. We can conclude that $\alpha<0$ if and only if:

$$cD\beta^2 + q_2 c > q_1 kn_0, \tag{14}$$

which can be considered as a necessary and sufficient condition for stability. The above condition has a better choice to be violated when the wavenumber β of the Fourier mode decreases to zero. In fact, if:

$$cq_2 < q_1 kn_0, \tag{15}$$

equation (14) will always be violated for wave numbers β close to zero. Therefore, instability arises as a product of long wavelength perturbations (Figure 2b).

Physically, condition (15) implies that strain localization will occur if the motility c of the strainions or the decay rate q_2 of the heat concentration are small or, inversely, if the rate of heat production q_1 or the thermotaxis coefficient k are large. The above conclusions may give some hints to explain the relatively high stability of carbon nanotubes as compared, e.g., to golden nanowires.

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