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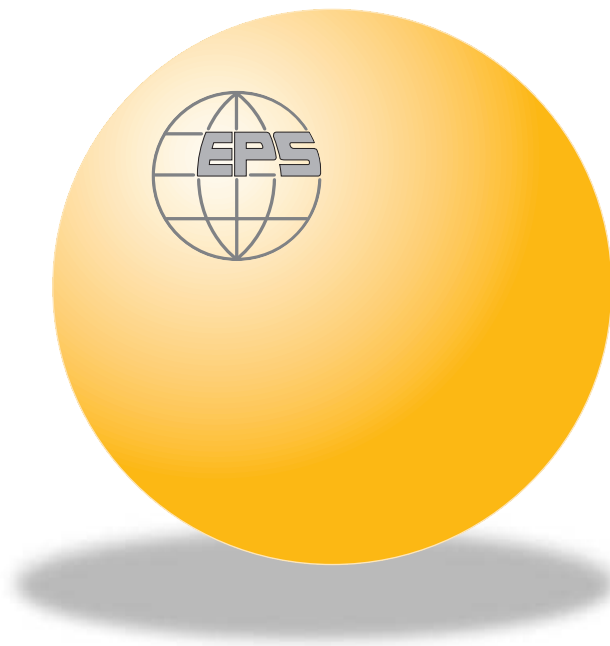
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Subscription 2004

24 issues - Vol. 65-68 (6 issues per vol.)

ISSN: 0295-5075 - ISSN electronic: 1286-4854

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Continuum mesoscale theory inspired by plasticity

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Abstract. – We present a simple mesoscale field theory inspired by rate-independent plasticity that reflects the symmetry of the deformation process. We parameterize the plastic deformation by a scalar field which evolves with loading. The evolution equation for that field has the form of a Hamilton-Jacobi equation which gives rise to cusp-singularity formation. These cusps introduce irreversibilities analogous to those seen in plastic deformation of real materials: we observe a yield stress, work hardening, reversibility under unloading, and cell boundary formation.

We call it plasticity when materials yield irreversibly at large external stresses. Macroscopically, plasticity is associated with three qualitative phenomena. To a good approximation, there is a threshold called the *yield stress* below which the deformation is reversible (see fig. 1). A material pushed beyond its yield stress exhibits *work hardening*, through which the yield stress increases to match the maximum applied stress. Finally, the deformed crystal develops patterns, such as the *cell structures* observed in fcc metals [1–3]. While much is known about all three phenomena, a quantitative understanding based on mesoscopic continuum theory would be welcome —especially if it connects to microscopic properties of the atomic interactions in the material. In this paper, we will discuss a simple scalar field theory which naturally exhibits these three key features of plasticity. We do not have a connection to microscopic properties, and do not claim to model in detail plasticity in real materials. However, we believe that a continuum description of plasticity should share the key feature of our model equation: a transition between reversible and irreversible deformation is generated by singularities which occur at finite stress.

There are a vast number of approaches to modeling plastic flow in metals —quantum, atomistic, motion of single dislocations, motion of many dislocations, continuum theories of dislocation densities, slip system theories, work hardening theories.... Reviewing even only the basic ideas of these models is beyond the scope of this paper. Three of them, however,
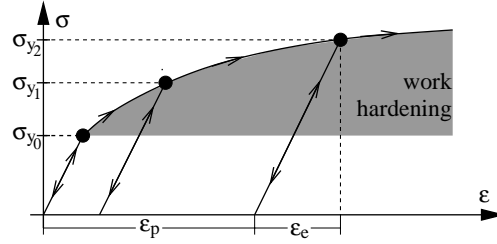

Fig. 1 – Generic stress-strain relation. For stress σ below the critical yield stress σ_{y_0} the deformation is elastic and reversible. Further deformation results in plastic deformation and work hardening, *i.e.* the yield point (bullet) moves to higher stress. The strain ε is partly due to reversible elastic deformation ε_e and partly due to irreversible plastic deformation ε_p.

directly inspired our approach. 1) Theories based on the differential geometry of the Burgers vector density torsion tensor [4, 5]. These elegant mathematical descriptions of the state of the material need to be supplemented by a similarly sophisticated dynamical evolution law —especially for the non-equilibrium problem of plastic flow. The torsion tensor theories are typically dismissed by the engineering community because they ignore the large majority of geometrically unnecessary dislocations which cancel out in the macroscopic Burgers vector density. It is not clear that this cancellation arises on the sub-grain mesoscale we study, but in this work we use a simpler scalar order parameter. 2) Macroscale engineering theories of plasticity, and, in particular, the recent strain gradient theories [6]. Their use of symmetry to constrain the form of the evolution laws is echoed in our approach. Their explicit incorporation of a yield surface is clearly appropriate on the macroscale, but is unsatisfactory for a condensed-matter physicist. In our model, the yield surface emerges naturally from the evolution laws through the development of cell structures on the mesoscale. 3) Theories which attempt to coarse-grain the complex rearrangement dynamics of atoms [7,8] or dislocations [9] to develop continuum plasticity theories. Any such description will introduce a field which describes the local state of the material as it evolves during deformation. Even though the microscopic dynamics of dislocations is understood to a large extent, coarse-graining the microscopic dynamics has not been successful up to now.

    We are going to study the following evolution equation for a scalar field which parameterizes rate-independent plastic deformation:

$$\frac{\partial \Psi}{\partial t} = \frac{\partial S_{ij}}{\partial t} \nabla_i \Psi \nabla_j \Psi. \tag{1}$$

We use Einstein's convention, summing over repeated indices. The plastic deformation is assumed not to depend on volume changes and the evolution depends only on the deviatoric stress $S_{ij} = \sigma_{ij} - \frac{1}{3}\sigma_{kk}\delta_{ij}$, with σ_{ij} the full stress tensor. There are two motivations to study this equation in the context of plasticity theory.

    First, we can derive this evolution equation as one of the leading terms in a long-wavelength expansion of a general local evolution equation for Ψ which respects the symmetries and the rate invariance of the loading process. However, there is *a priori* a term of the same order $\frac{\partial S_{ij}}{\partial t} \nabla_i \nabla_j \Psi$ which turns out to be highly singular since it leads to finite-time divergences of the field Ψ. Although rate-independent (creep) terms such as $\nabla^2 \Psi$ (and higher-order derivatives) should regularize these divergences, we prefer to discard these singular terms altogether in the present discussion and focus on eq. (1) which, as we now show, already contains a rich phenomenology. We will indeed show later that eq. (1) can be transformed into a Hamilton-Jacobi equation which is known to form finite-time singularities. These singularities are the

second reason to study this equation, since they can be related to the onset of irreversibility and to dislocation structure formation. Second, Hamilton-Jacobi equations are also related to conservation laws as studied in the context of traffic jams and at least on a naive level there is a similarity between traffic jams and dislocation entanglement [10, 11].

We will focus on so-called proportional loading paths (such as those used in shear and tension tests, where the loading direction does not change), where the stress $S_{ij}(t) = \sigma(t)\hat{S}_{ij}$. Thus in eq. (1) we change variables from time t to stress amplitude σ:

$$\frac{\partial \Psi}{\partial \sigma} = \hat{S}_{ij} \nabla_i \Psi \nabla_j \Psi. \tag{2}$$

In the form of eq. (2), we see the key challenge in formulating laws of rate-independent plasticity: the equations appear to be manifestly reversible. Increasing and then reducing σ will naively leave the material in the original state. The engineers bypass this problem by formulating their theories not in terms of order parameter fields, but directly in terms of a yield surface (corresponding to step functions $\Theta(\sigma - \sigma_y)$ in the equations of motion). However, eq. (2) is a Hamilton-Jacobi equation (closely related to the multidimensional anisotropic Burgers equation, see [12]) which develops cusp-shaped singularities at finite σ even for smooth initial conditions. At these singularities, as numerically illustrated below, information and thus reversibility is lost. The stress at which the first singularities form has many features of a yield surface, as we will show later.

After the formation of singularities, the solution of eq. (2) is not unique and one has to find a weak solution which regularizes the singularities. As mentioned above, the assumption of a rate-independent behavior discards creep relaxation effects which enter eq. (1) in form of a diffusion term $\nabla_k \nabla_k \Psi$ with a rate-independent coefficient. Such a term with an infinitesimally small prefactor is enough to regularize the singularities and one gets the so-called viscosity solution, which we will consider in the following.

We solve eq. (2) numerically on a finite-difference grid using the problem-solving environment CACTUS 4.0 [13]. The initial condition was a Gaussian random field with amplitude and correlation length one. The convolution was performed in Fourier space using the fast Fourier transform package FFTW 2.1.3 [14]. We use an essentially non-oscillatory (ENO) scheme in combination with Godunov's method to minimize numerical damping [15]. The algorithm is proven to converge to the viscosity solution. The numerical grid has periodic boundary conditions; in one dimension (1D) the length of the system is 100 and the system had 4084 points; in two dimensions (2D) the size of the system is 25^2 and the grid was 1016^2. The three-dimensional (3D) simulation cell was 12.5^3 and the grid size 264^3. The ENO stencil width was 4 in one and 5 in 2D and 3D, respectively, and the time stepping scheme is a simple explicit Euler scheme with a time step $\delta\sigma = 10^{-3}$. The system is cycled by unloading beginning at various points σ_n and reloading at somewhat above zero stress (to reduce the effect of numerical damping).

Figure 2 shows the evolution of the Burgers equation in 1D, corresponding to eq. (2) with $S_{ij} = 1$. The cusps develop in the valleys at $\sigma \approx 0.3$, and the unloading and reloading paths are both shown. Since the cusps disappear immediately upon unloading, the order parameter evolution is reversible until the stress grows to match the previous maximum, so our model exhibits work hardening.

Finally, fig. 3 shows the cusp locations in two cross-sections of a 3D simulation with $\hat{S}_{xx} = 2/3$, $\hat{S}_{yy} = \hat{S}_{zz} = -1/3$, and $\hat{S}_{ij}$ zero otherwise, appropriate to a tension test. We see that the cusps form nearly flat 1D interfaces separating cell-like volumes. While the cut parallel to the loading direction (a) shows the expected asymmetry, the cut perpendicular to the loading direction (b) shows an isotropic hexagonal cell structure. Simulations under shear
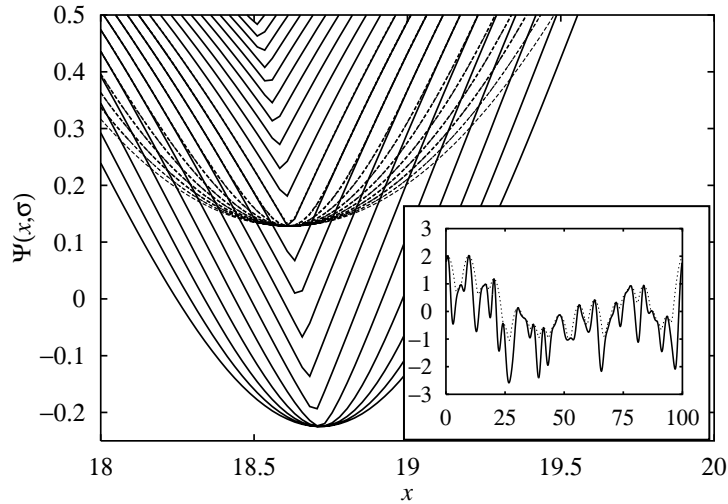
Fig. 2 – Blow-up of the region $18 < x < 20$ from our 1D simulation. The solid lines represent $\Psi(x)$ for σ values 0.1 apart starting at $\sigma = 0$, with curves further up having larger σ. The dashed lines are $\Psi(x)$ while unloading and the dotted ones while reloading. The dotted lines are hardly visible because in the reversible region they lie on top of the dashed ones. At the cusps, the spatial discretization is visible. The inset shows the initial (solid) and final (dashed) configuration of the whole system, *i.e.* for $\sigma = 0$ and 6.

in 2D ($\hat{S}_{xx} = 1/2$, $\hat{S}_{yy} = -1/2$, and zero otherwise) show similar cusps to fig. 3(a). These morphologies are reminiscent of cell structures formed in hardened fcc metals [3].

The size distribution of the cells depends on the initial conditions and the cells coarsen in contrast to the cell refinement observed in experiments. Moreover, the cell walls in our model blur upon unloading, (see fig. 2), much more than is seen experimentally. It is clear that these effects call for a more realistic extension of the present model, but we believe that the emergence of *spatial structures*, coupled with finite-stress singularities which lead to irreversibility, is a generic feature which will be shared by a more elaborated non-linear field description of plasticity.

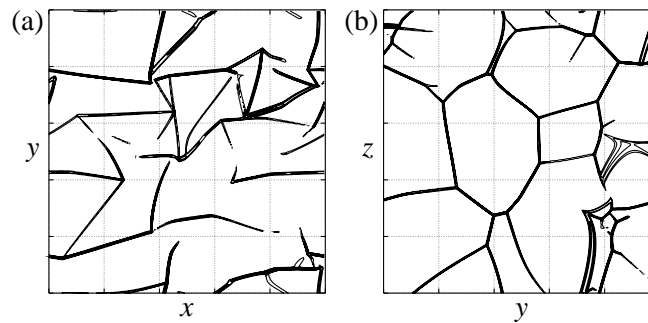We now wish to calculate a scalar, *e.g.*, the total plastic strain, from the Ψ field which

Fig. 3 – Location of the singularities for tension test at $\sigma = 1$ in (a) the xy-plane and (b) yz-plane, that is parallel and perpendicular to the loading direction, respectively. The lines are contour lines $\hat{S}_{ij}\nabla_i\nabla_j\Psi = 1.5, 3, 6, 9, \ldots$. Our symmetry analysis does not provide us with a physical interpretation for Ψ.
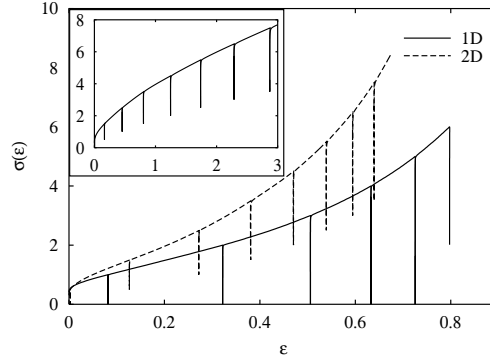
Fig. 4 – Stress-strain relation according to eq. (3) for our 1D (solid line) and 2D (dashed line) model, and for our 2D model with a stress-dependent prefactor $1 + 0.25\, S_{mn}\, S_{mn}$ (inset).

illustrates the transition from reversible to irreversible behavior in a similar way as the stress-strain relation in fig. 1. The term we are going to calculate and which we will call strain is

$$\frac{\partial \varepsilon}{\partial \sigma} = \sigma \hat{S}_{k\ell} \big\langle (\nabla_k \Psi)(\nabla_\ell \Psi) \boldsymbol{\nabla}^2 \Psi \big\rangle. \tag{3}$$

The angle brackets are spatial averages. There are two reasons for focusing on this term.

First it is sensitive to the formation of cusp singularities. At the cusp, the second derivative gives a delta-function. Hence, the appearance of singularities will greatly affect the strain.

Second, the term in eq. (3) is part of a gradient expansion. We assume (as common among engineers) that the deformation is in the direction of the applied stress S_{ij}. If we expand the strain rate $\partial \varepsilon / \partial t$ to second order in S_{ij} and fourth order in gradients, the term in eq. (3) is one of the terms. Other terms are either insensitive to the singularities or they are surface terms (which would give zero average strain since we use periodic boundary conditions). There is, however, one extra term in such an expansion, which is highly singular, namely $S_{ij} \frac{\partial S_{k\ell}}{\partial t}(\nabla_k \nabla_\ell \Psi) \boldsymbol{\nabla}^2 \Psi$. This term would lead to a delta-function squared at a cusp, which we again neglect.

Figure 4 shows the resulting stress-strain curves for our plasticity theory. In 1D and 2D the term in angle brackets in eq. (3) is a total divergence: it is proportional to $\nabla_x (\nabla_x \Psi)^3$ and $\nabla_x [(\nabla_x \Psi)^3/3 - (\nabla_x \Psi)(\nabla_y \Psi)^2] - \nabla_y [(\nabla_y \Psi)^3/3 - (\nabla_y \Psi)(\nabla_x \Psi)^2]$ in 1D and 2D, respectively. This implies that $\langle \partial \varepsilon_{ij} / \partial t \rangle = 0$, explaining why the unloading curves are vertical in fig. 4. Plastic deformation occurs on the main loading curve because the cusps act as sources for the total divergence term. (We do not show stress-strain curves for the 3D simulations. Because of numerical limitations the results would be governed by finite-size effects, *i.e.*, too few cells in the sample volume. Qualitatively the stress-strain curves look similar.)

In the inset of fig. 4 we added a stress-dependent prefactor to eq. (3) in order to change the curvature of the stress-strain curve and make it look more similar to fig. 1. This is to demonstrate that the upward bending of the stress-strain curve is more related to the interpretation of the field Ψ rather than to the evolution equation (1). The form of the initial conditions could also influence the shape of the stress-strain curve considerably, in particular the onset of instabilities.

Note that the point where the unloading curves meet the main stress-strain curve moves to higher stresses for increasing plastic deformation, *i.e.*, the yield surface moves to higher stresses for higher deformation. In other words, our model equation shows work hardening. The work hardening is generic to the evolution equation and independent of the formula for

the plastic strain, since the yield surface (*i.e.*, the formation of singularities) moves to higher and higher stresses in eq. (1).

The simple Hamilton-Jacobi equation (or anisotropic Burgers equation) (1) together with the plastic strain as calculated from eq. (3) forms a theory which generically has all three mysterious features of plasticity, namely an evolving yield surfaces, cell structure formation (with the proper cell morphology for the given loading), and work hardening. However, as already mentioned, there are significant differences between our model and real plasticity. The cell structure in our model coarsens while it refines in real systems; also, the cell walls blur upon unloading in our model. Some of these shortcomings might be related to the choice of the viscosity solution as weak solution, to the absence of noise in our evolution equation, or the choice of initial conditions. They may also be due to our choice of a scalar order parameter: we are exploring theories more closely tied to the microscopics, based on the dislocation density tensor [16].

The main point we want to make here is that an evolving yield surface and work hardening-like behavior is generated generically by the formation of cusp-singularities in Hamilton-Jacobi equations (and probably other types of singularities in different evolution equations). The analogy of the singularities in our model with the cell walls is only qualitative, but it suggests that a mesoscale continuum theory will have cell walls as singular structures, that will be central to work hardening and an evolving yield surface. We hope that the ideas presented in this paper will motivate further research in that direction.

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