

Mesoscale Theory of Grains and Cells: Crystal Plasticity and Coarsening

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Crystals with spatial variations in their axes naturally evolve into cells or grains separated by sharp walls. At high temperatures, polycrystalline grains form from the melt and coarsen with time: the dislocations can both climb and glide. At low temperatures under shear the dislocations (which allow only glide) form into cell structures. We present here a mesoscale theory of dislocation motion. It provides a quantitative description of deformation and rotation, grounded in a microscopic order parameter field exhibiting the topologically conserved quantities. The topological current of the Nye dislocation density tensor is derived from a microscopic theory of glide driven by Peach-Koehler forces between dislocations using a simple closure approximation. The resulting theory is shown to form sharp dislocation walls in finite time, both with and without dislocation climb.

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Crystals, when formed or deformed, relax by developing walls. Common metals (coins, silverware) are polycrystalline: the atoms locally arrange into grains each with a specific crystalline lattice orientation, separated by sharp, flat walls called *grain boundaries*. When metals are deformed (pounded or permanently bent) new *cell walls* form inside each grain [1–3]. Until now, our only convincing understanding of why crystals form walls has been detailed and microscopic. Our new theory provides an elegant, continuum description of cell wall formation as the development of a *shock front*—a phenomenon hitherto associated with traffic jams and sonic booms.

Continuum theories of dislocation dynamics are not new [4–7]. Various approaches have been used to study dislocation pattern formation. Simplified diffusion models have been used to describe persistent slip bands [8], dislocation cell structures during multiple slip [9], and dislocation vein structures [10]. Models similar in spirit to ours have recently been analyzed both for single slip [11–13] and in three dimensions [14]. None of these approaches have yielded the sharp, wall-like singularities characteristic of grain boundaries and deformation-induced cell structures (see, however, [15]).

Continuum plasticity theory, as used in practical engineering codes, describes the deformation gradient ($\partial_i u_j$, for displacement field \mathbf{u}) as the sum $\partial_i u_j = \beta_{ij}^E + \beta_{ij}^P$ of an elastic, reversible distortion β^E and a permanent plastic distortion β^P . The plastic distortion involves the creation of microscopic dislocations and cannot be written as a gradient of a single-valued displacement field. Integrating around a loop L enclosing a surface S , the change in such a hypothetical plastic distortion field $\Delta \mathbf{u}^P$ can be written using the Stokes theorem as

$$\Delta u_j^P = - \oint_L \beta_{ij}^P dx_i = - \int_S \varepsilon_{ilm} \frac{\partial \beta_{mj}^P}{\partial x_l} dS_i = \int_S \rho_{ij} dS_i, \quad (1)$$

where the Nye dislocation density tensor

$$\rho_{ij}(\mathbf{x}) = -\varepsilon_{ilm} \frac{\partial \beta_{mj}^P}{\partial x_l} = \sum_{\alpha} t_i^{\alpha} b_j^{\alpha} \delta(\xi^{\alpha}) \quad (2)$$

measures the net flux of dislocations α , tangent to \mathbf{t} , with Burgers vector \mathbf{b} , in the (coarse-grained) neighborhood of \mathbf{x} . The microscopic statement that dislocations cannot end implies $\partial_i \rho_{ij} = 0$, so the time evolution must be given in terms of a current [6,7,16] \mathbf{J} : $\partial \rho_{ij} / \partial t = -\varepsilon_{ilm} \partial J_{mj} / \partial x_l$. From Eq. (2) we see that [17]

$$J_{ij} = \partial \beta_{ij}^P / \partial t. \quad (3)$$

Thus the natural physicist's order parameter (the topologically conserved dislocation density ρ) is a curl of the common engineering state variable (the plastic distortion field β^P). The focus of our Letter will be the derivation of an evolution law (3) appropriate for scales large compared to the atoms but small compared to the cell structures and grain boundaries.

Notice that we consider only the *net* density of dislocations. We ignore the geometrically unnecessary dislocations (those with opposing Burgers vectors which cancel out in the net dislocation density) because they do not affect the long-range strain fields or the misorientations at grain boundaries and cell walls. Macroscopically they are known to dominate dislocation entanglement and work hardening, and are included in previous continuum theories of plasticity [8,11–13,18,19]. Much of the macroscopic cancellation in net dislocation density comes from the near alternation of the net rotations in the series of cell walls [20]. Our focus on the subcellular, subgrain length scales and our current omission of dislocation tangling make keeping only the net dislocation density natural for our purposes. We also do not explicitly incorporate a yield surface, because we hope eventually to explain work hardening and yield surfaces as properties which emerge from the intermediate length-scale theory.

We motivate our evolution law from the microscopic Peach-Koehler force on a section of a dislocation line due

to the stress field $\boldsymbol{\sigma}$ present at that point: $f_i^{\text{PK}} = -\varepsilon_{ijk}t_j b_l \sigma_{kl}$. The current \mathbf{J} of a single dislocation moving with velocity \mathbf{v} is $J_{ij} = \varepsilon_{ilm}t_l b_j v_m \delta(\xi)$. If we treat dislocation glide and climb on an equal footing (a crude model for metals at high temperatures), the dislocation will move in the direction of the applied force $\mathbf{v} \propto \mathbf{f}^{\text{PK}}$. For a single dislocation, tuning the climb component with a parameter λ , we find

$$J_{ij} = D \left[\varepsilon_{ilm}t_l b_j \varepsilon_{mpq} \sigma_{pr} t_q b_r \delta(\xi) - \frac{\lambda}{3} \delta_{ij} \varepsilon_{klm} t_l b_k \varepsilon_{mpq} \sigma_{pr} t_q b_r \delta(\xi) \right]. \quad (4)$$

Here D is a materials constant with units of $[\text{length}]^2 \times [\text{time}]/[\text{mass}]$ giving the mobility of dislocation glide. At

$$\rho_{ijkm}^{(4)} = \sum_{\alpha} t_i^{\alpha} b_j^{\alpha} t_k^{\alpha} b_m^{\alpha} \delta(\xi^{\alpha}) \simeq C \left[\sum_{\alpha} t_i^{\alpha} b_j^{\alpha} \delta(\xi^{\alpha}) \right] \left[\sum_{\alpha'} t_k^{\alpha'} b_m^{\alpha'} \delta(\xi^{\alpha'}) \right] = C \rho_{ij} \rho_{km}, \quad (6)$$

where C has units of distance. The resulting evolution law for the plastic distortion tensor is

$$\frac{\partial \beta_{ij}^{\text{P}}}{\partial t} = \frac{CD}{2} \left[(\sigma_{ic} \rho_{ac} - \sigma_{ac} \rho_{ic}) \rho_{aj} - \frac{\lambda}{3} \delta_{ij} (\sigma_{kc} \rho_{ac} - \sigma_{ac} \rho_{kc}) \rho_{ak} \right], \quad (7)$$

where $\boldsymbol{\rho}$ is a curl of $\boldsymbol{\beta}^{\text{P}}$ [Eq. (2)], and the stress $\boldsymbol{\sigma}$ (due to the long-range fields of the other dislocations) is written in Fourier space as [22]

$$\begin{aligned} \tilde{\sigma}_{ij}(\mathbf{k}) &= K_{ijkl}(\mathbf{k}) \tilde{\rho}_{kl}(\mathbf{k}), \\ K_{ijkl}(\mathbf{k}) &= -\frac{i\mu k_m}{k^2} \left[\varepsilon_{ilm} \delta_{jk} + \varepsilon_{jlm} \delta_{ik} + \frac{2\varepsilon_{klm}}{1-\nu} \left(\frac{k_i k_j}{k^2} - \delta_{ij} \right) \right]. \end{aligned} \quad (8)$$

For simplicity, we present solutions to our three-dimensional theory for the special case of systems where the dislocation density varies only along one and two dimensions. In one dimension with variations only along \hat{z} , our theory becomes local, with stress

$$\boldsymbol{\sigma}(z) = -\mu \begin{pmatrix} \frac{2}{1-\nu}(\beta_{xx}^{\text{P}} + \nu\beta_{yy}^{\text{P}}) & \beta_{xy}^{\text{P}} + \beta_{yx}^{\text{P}} & 0 \\ \beta_{xy}^{\text{P}} + \beta_{yx}^{\text{P}} & \frac{2}{1-\nu}(\nu\beta_{xx}^{\text{P}} + \beta_{yy}^{\text{P}}) & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad (9)$$

Nye dislocation tensor

$$\rho_{xj} = \partial_z \beta_{yj}^{\text{P}}, \quad \rho_{yj} = -\partial_z \beta_{xj}^{\text{P}}, \quad \rho_{zj} = 0, \quad (10)$$

and evolution law

$$\frac{\partial \boldsymbol{\beta}^{\text{P}}}{\partial t} = -F(\boldsymbol{\beta}^{\text{P}}) \frac{\partial \boldsymbol{\beta}^{\text{P}}}{\partial z}, \quad (11)$$

with

$\lambda = 0$, climb and glide have equal mobilities, and at $\lambda = 1$, \mathbf{J} is traceless and hence only glide is allowed. Coarse graining over many dislocations,

$$J_{ij} = D_{ijkmpqrs} \sigma_{pq} \rho_{kmrs}^{(4)}, \quad (5)$$

where $D_{ijkmpqrs} = D/2[\delta_{iq} \delta_{jm} \delta_{kr} \delta_{ps} - \delta_{ir} \delta_{jm} \delta_{kq} \delta_{ps} - \lambda/3(\delta_{ij} \delta_{mq} \delta_{kr} \delta_{ps} - \delta_{ij} \delta_{mr} \delta_{kq} \delta_{ps})]$, is an eighth rank isotropic tensor specific to Peach-Koehler model, and $\rho_{kmrs}^{(4)}$ is a higher order Nye dislocation tensor. Thus that the evolution of $\boldsymbol{\rho}$ depends upon the new object $\boldsymbol{\rho}^{(4)}$.

We now need to perform a *closure approximation*, writing $\boldsymbol{\rho}^{(4)}$ in terms of $\boldsymbol{\rho}$ (as in Hartree-Fock and in theories of turbulence). The only choice $\boldsymbol{\rho}^{(4)} \rightarrow \boldsymbol{\rho} \otimes \boldsymbol{\rho}$ that guarantees a decrease of elastic energy with time [21] is

$$\begin{aligned} F(\boldsymbol{\beta}^{\text{P}}) &= -\frac{\partial w(\boldsymbol{\beta}^{\text{P}})}{\partial z} \\ &= -CD\mu \frac{\partial}{\partial z} \left[\frac{1}{2}(\beta_{xy}^{\text{P}} + \beta_{yx}^{\text{P}})^2 + (\beta_{xx}^{\text{P}2} + \beta_{yy}^{\text{P}2}) \right. \\ &\quad \left. + \frac{\nu}{1-\nu}(\beta_{xx}^{\text{P}} + \beta_{yy}^{\text{P}})^2 \right]. \end{aligned} \quad (12)$$

Interestingly, $w(\boldsymbol{\beta}^{\text{P}})$ is the linear elastic energy density of the system, the effective force $F(\boldsymbol{\beta}^{\text{P}})$ is proportional to the z component of the Peach-Koehler force, and the rate of change of the elastic energy density is simply $-F^2(\boldsymbol{\beta}^{\text{P}})$ (so the energy decreasing condition is explicit).

Our equation for $\boldsymbol{\beta}^{\text{P}}$ in one dimension is hyperbolic: the method of characteristics may be applied, where the characteristics are the parametrized curves $(t(s), z(s))$ with $dt/ds = 1$, $dz/ds = F(\boldsymbol{\beta}^{\text{P}})$. Along these curves,

$$\frac{d\boldsymbol{\beta}^{\text{P}}}{ds} = \frac{dt}{ds} \frac{\partial \boldsymbol{\beta}^{\text{P}}}{\partial t} + \frac{dz}{ds} \frac{\partial \boldsymbol{\beta}^{\text{P}}}{\partial z} = \frac{\partial \boldsymbol{\beta}^{\text{P}}}{\partial t} + F(\boldsymbol{\beta}^{\text{P}}) \frac{\partial \boldsymbol{\beta}^{\text{P}}}{\partial z} = 0, \quad (13)$$

implying ([from Eq. (11)] that $\boldsymbol{\beta}^{\text{P}}$ is constant along the characteristics. As with many hyperbolic systems, we observe shock formulation in finite time. Our analytic analysis of the shock asymptotics (in preparation) exhibits the jump in $\boldsymbol{\beta}^{\text{P}}$, wall in $\boldsymbol{\rho}$, and stress jump described numerically below, with a $1/\sqrt{t}$ time dependence for the surrounding continuum $\boldsymbol{\beta}^{\text{P}}$.

We simulate systems of spatial extent L in one or two dimensions, with periodic boundary conditions and no external stress. The initial plastic distortion field $\boldsymbol{\beta}^{\text{P}}$ is a Gaussian random field with mean-square amplitude β_0^{P} and root-mean-square decay length approximately $L/16$. In one dimension, we use the upwind scheme [23] as implemented by Press *et al.* [24]. In two dimensions, we calculate $\boldsymbol{\sigma}$ using Fourier methods and regularize our equations by adding a fourth-order numerical viscosity $-K\nabla^4 \beta_{ij}^{\text{P}}$ to Eq. (7). (A second-order viscosity $\nabla^2 \beta_{ij}^{\text{P}}$ was not as suc-

cessful in suppressing the instabilities.) In one dimension, we have checked that the upwind scheme produces the same solution as the viscosity regularization. Unlike shock waves in fluids, where conservation laws tell us that the upwind or viscosity solution is the correct one, here the dynamics of the walls is not determined by the continuum theory. (We speculate that the wall dynamics regularization may be nontrivial and stochastic, emerging out of avalanches and critical depinning phenomena on subcell length scales—observed both experimentally [25] and theoretically [26] in systems with only one active slip system.)

Figure 1 shows the final state of the plastic distortion β^P in a one-dimensional system evolving under dislocation glide only (corresponding to plastic deformation, which experimentally leads to cell structure formation). Jump singularities in β^P form after a short time, representing a wall of dislocations and an abrupt change in lattice orientation. The cell walls in our model are not grain boundaries, because they do not correspond to pure, simple rotations (they do not satisfy the Frank conditions [27]). There is a jump in the stress across each cell wall: the glide component of the forces from the two neighboring cells on ρ in a wall is equal, opposite, and compressive. Our model therefore predicts that the initial formation of cell walls during low-temperature plastic deformation is driven by a stress jump due to noncancellation of the stress field of the constituent dislocations. As our system evolves, new cell walls form (intriguingly similar to the cell refinement seen experimentally [28,29]) and the existing cell walls evolve to reduce their stress jumps.

Figure 2 shows the evolution of the plastic distortion in a system allowing both glide and climb, corresponding to high-temperature annealing of a plastically deformed structure. Here the initial singularities again are not grain boundaries, but walls of dislocations with net stress jumps. These walls then move and coalesce in response to the net

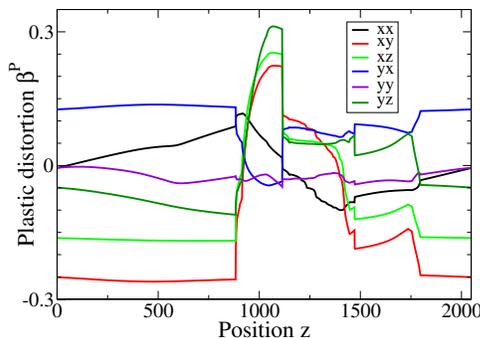


FIG. 1 (color online). Plastic distortion tensor component β^P_{ij} in one dimension allowing only glide motion, after time $t = 20L^2/D\mu$, with 2048 mesh points. The shocks or jumps in the values correspond to the cell walls. A stress-free wall (satisfying the Frank conditions) here would have no jump in β^P_{xx} , β^P_{yy} , or $\beta^P_{xy} + \beta^P_{yx}$.

force due to other dislocations, coarsening the resulting grain boundary structure.

Figure 3 shows the final state of β^P in a two-dimensional plasticity simulation (with glide and not climb). Notice the formation of sharp walls (mathematically demonstrated above only in one dimension). These walls separate relatively unstrained regions which we identify with the cells formed during plastic deformation. As in the one-dimensional simulations, the cell walls formed at short times have stress jumps.

Generically we expect our model to form sharp walls in finite time. Special initial conditions, however, may not form walls. Indeed, the case of a single-slip system does not form singularities within our model—perhaps explaining why cell wall formation is not observed in stage I hardening or in dislocation-dynamics studies of single slip in two dimensions otherwise similar to our approach [11–13].

Our dislocation-dynamics theory is minimalist: it ignores many features (geometrically unnecessary dislocations [11], slip systems [30], dislocation tangling, yield surfaces, nucleation of new dislocations, etc.) that are known to be macroscopically important in real materials. It does incorporate cleanly and microscopically the topological constraints, long-range forces, and energetics driving the dislocation dynamics. As hypothesized by the low-energy dislocation structures approach [31,32], we find that a dynamics driven by minimizing energy (omitting tangling and nucleation) still produces cell boundary structures. Finally our theory, to our surprise, initially forms sharp walls that are not the usual zero-stress grain boundaries.

In condensed-matter physics, crystals are anomalous. Most phases (liquid crystals, superfluids, superconductors, magnets, etc.) respond smoothly in space when strained. Crystals, when rotationally strained, form sharp walls separating cells or grains. Our analysis suggests that the formation of these walls can be understood as a shock formation in the dislocation dynamics.

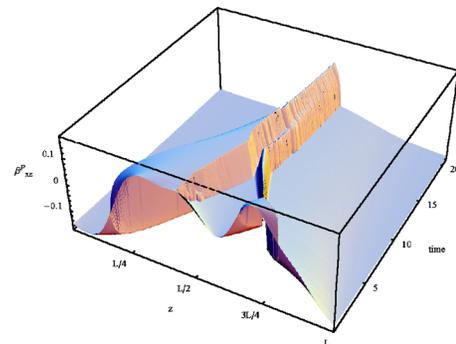


FIG. 2 (color online). The xz component of the plastic distortion tensor in one dimension up to time $t = 22L^2/D\mu$, with 2048 mesh points. The evolution allows both glide and climb motions. The walls move and coalesce until only a single wall survives.

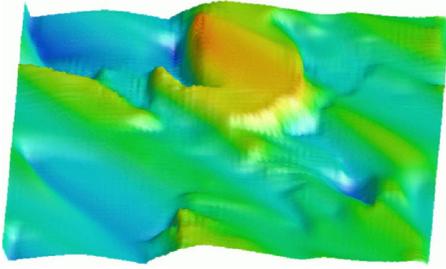


FIG. 3 (color online). The yz component of the plastic distortion tensor allowing only glide, in two dimensions after time $t = 9.15L^2/D\mu$.

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$$J_{ij}^{vM} = \kappa \left(\sigma_{ij} - \frac{\sigma_{kk}}{3} \delta_{ij} \right) \Theta \left(\frac{1}{2} \sigma_{pq} \sigma_{pq} - \frac{1}{3} \sigma_{pp} \sigma_{qq} - \frac{1}{3} \sigma_Y^2 \right),$$

where $\Theta(\cdot)$ is the Heaviside step function. The von Mises law has dislocation flow that is independent of the existing net dislocation density: it is appropriate on macroscopic scales where the geometrically unnecessary dislocations are thought to dominate plasticity.

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