Modeling energetics and noise in dislocation patterning

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(Received 22 August 2004; revised manuscript received 30 November 2005; published 13 January 2006)

We explore the underlying physics of dislocation ordering in deforming metals, where we focus on the competing role of energy relaxation and the fluctuations (noise) in the local stress field. We investigate the competition by employing a simple two-dimensional model that exhibits the essential physics, while avoiding extraneous mechanisms that might cloud the issues. We show that noise and energetics are equally important in determining the final state of the system. Quantitative functions for the energetic driving force for ordering and the resistive force owing to the noise are developed that balance one another at the relaxed state. These features follow from the system being scale invariant, with power law dependencies of the macrovariables on the number of relaxing dislocations.

DOI: 10.1103/PhysRevB.73.024104 PACS number(s): 61.72.Bb

I. INTRODUCTION

Perhaps the most intractable aspect of developing a theory of the deformation in metals is to understand the physics behind the formation of the partially ordered dislocation cells delineated by a rather vague three-dimensional (3D) network of dislocation walls that appear as the deformation proceeds.[1] This ordering takes place while the system is far from thermal equilibrium and in the presence of very large fluctuations, or noise, in the relevant variables.[2–4] The noise is such a striking feature of the system that Hähner has proposed that the transition to the cell structure should be considered primarily noise generated.[2,4] We have also presented support for this view.[5]

The purely stochastic type of analysis by Hähner and others[2–5] neglects, however, all effects (except for the annihilation of unlike dislocations) owing to the interaction energy (or forces) between the dislocations. We know, however, that the interactions between dislocations are large and anisotropic[6] and that these interactions lead to the formation of a strong local order.[7–9]

The goal of this paper is to directly examine the relative roles of the interaction forces and the noise in the ordering of dislocations. We will show that the noise and energy drive the system in opposite directions relative to the state of order and come into balance at the relaxed state, in a somewhat analogous way that thermal fluctuations and cohesive energy balance each other in thermodynamic systems.

It is important to be clear about what we mean by noise in this paper. We are not talking about thermal noise, which can be viewed as an external fluctuating force acting on particles in a system. Thermal noise is additive, in that the fluctuating forces acting on a variable are independent of that variable. Thermal noise is relatively unimportant in systems of dislocations, however, because elastic interactions are so much larger in magnitude than the thermal forces.[10] (This is not to say that temperature effects are not important; they are critical in defining atomistic-level activated events, such as climb, cross slip, etc.).

In contrast with thermal noise, the dominant fluctuations in the forces in a system of dislocations are self-generated and arise from the long-ranged elastic interactions between the dislocations themselves. These fluctuations are tied self-consistently to the evolving structure of the dislocations and are thus not independent variables, as the temperature is in thermodynamics. To be more specific, consider the force on a mobile dislocation as it moves along its slip plane. The highly anisotropic nature of the interactions between dislocations leads to a frustration between forming locally ordered structures (driven by the attractive regions of the interactions) and nonordered structures (driven by the repulsive regions of the interactions). This frustration arises from the stochastic distribution of orientations between neighbors and leads to large fluctuations in the forces acting on the dislocations. A measure of these fluctuations (the standard deviation of the local stress field) will be employed below as a concrete definition of the noise. We note that this measure of noise describes forces that depends on the variables upon which they act (the dislocation positions) and thus is generally referred to as a multiplicative noise.[11] This definition of noise is consistent with that proposed earlier by Hähner.[3,12]

In the dislocation problem, there are actually several contributions to the frustration. The first is the constraint of a given dislocation to remain on a single slip plane, which means that the climb that would permit a uniform distribution of dislocations in the walls (the low energy configuration) is not allowed. A second contribution, arising from the angular dependence of the force law and described in the previous paragraph, frustrates complete wall formation irrespective of the distribution of dislocations within the walls. In our simple model, these are the major issues. In more complicated systems, there will be other contributions to the frustration. For example, when more than one Burgers vector is present, dipole formation is a form of frustration, and in 3D systems, entanglement is another form of frustration.

We explore in this paper the edge-ordering problem in the simplest possible model in which the features described above are dominant. The study is intended to throw light on the ordering observed in deforming systems, and to do so, we will simplify the actual deforming system, and reduce the problem to one where the interaction between "noise" and energy is central to the system, and all other aspects of dislocation behavior, such as annihilation, jog formation, multiple slip plane effects, etc. have been eliminated. The system

that does this most simply is that of 2D parallel edge dislocations with a single slip plane and single-signed Burgers vector.

We study the relaxation of an initially random configuration of dislocations. The relaxation case is not unrelated to steady-state deformation, because a deforming system does not respond in a continuous manner to the external stress, but with discrete stochastic strain bursts, or avalanches.[13,14] After each strain burst, the material in the vicinity of the strain burst relaxes until the stress builds up to the new local (and stochastic) critical stress. One of us has explored this behavior as a percolation process,[15] but here the focus is on the relaxation after a strain burst. The result of the percolation event will be the injection of a number of essentially (locally) randomly distributed new dislocations, which are added to the partially relaxed configuration resulting from the previous relaxation. So the situation after a percolation event in the actual deforming metal is not unlike the simplified annealing system explored here.

A final observation is that the system under study will be purely mechanical, with no overcoming of energy barriers by thermal fluctuations. Again, we simplify in order to understand, and can add additional complexity in later stages.

II. THE MODEL

We consider a system consisting of N edge dislocations, with Burgers vector $\vec{b}=b\hat{x}$, on a periodic square lattice in the xy plane with ($L=1000$) lattice sites on a side. The dislocation line direction is along the $\hat{z}$ direction, so the system is effectively two-dimensional. Since we ignore climb, motion is possible only in the $\pm\,\hat{x}$ direction. The dislocations are initially randomly distributed on the lattice. Periodic boundary conditions are assumed, which means that the square box with its dislocations is exactly replicated in each supercell of the lattice. Thus, the interaction of a given reference dislocation (the one on which the force is calculated) with a given neighbor dislocation is actually an interaction with an infinite wall of those neighbor dislocations along the $\hat{y}$ direction, with the repeat distance in the wall given by the supercell size. Each vertical wall is repeated in the $\hat{x}$ direction by additional walls, again separated by the super cell repeat distance. The force on a single dislocation in the presence of a wall extending infinitely in the $\pm\hat{y}$ direction is given by[6,7]

$$f_x = \frac{\pi\mu b^2}{L(1-\nu)} \frac{x[\cosh(2\pi x)\cos(2\pi y) - 1]}{[\cosh(2\pi x) - \cos(2\pi y)]^2}, \qquad (1)$$

where $x=(x_2-x_1)/L$ and $y=(y_2-y_1)/L$. (x_1,y_1) is the reference dislocation lattice coordinate and (x_2,y_2) is the lattice coordinate of the neighbor (or field) dislocation. Lattice rotations will be ignored. We normalize the expression in Eq. (1) such that $b=1$ and $\pi\mu/(1-\nu)=1$, where b is the Burgers vector, μ is the shear modulus, and ν is Poisson's ratio. Because of the periodic boundary conditions, there is an additional sum over the corresponding walls in each repeat supercell in the $\pm\hat{x}$ direction. We carry this (infinite) sum out to a distance of seven supercells in the $\pm\hat{x}$ direction, which leads to essentially complete convergence.

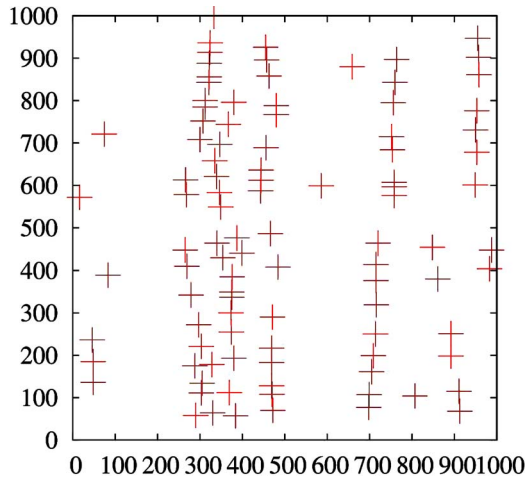

FIG. 1. (Color online) Output of a simulation for 100 relaxed dislocations. Considerable, but not complete, wall formation is apparent.

We sum the force on a reference dislocation from all its neighbors and move the reference dislocation one lattice spacing in the direction of the force. The calculation is repeated a few times (normally 10) with the neighbor dislocations remaining in their original positions. Finally, the (relaxation) calculation is repeated for each dislocation serving in turn as the reference dislocation and the whole process is repeated until convergence is attained. We have found that following this procedure leads to structures that are essentially equivalent to those obtained by other methods.[7,8] In Fig. 1 we show the relaxed positions of a system with $N=100$ dislocations. While there are reasonably well-defined walls, the result is clearly not at the absolute minimum of energy. Simulations starting with a different set of random positions would yield similar, but different, microstructures.

We characterize the magnitude of the fluctuations in the local forces acting on a dislocation (the noise) as the standard deviation of the distribution of the resolved shear stress on the slip plane. To calculate that quantity, we employ the relation between the standard deviation σ_a of a fluctuating quantity a and the average of the absolute value of that quantity $\langle|a|\rangle$,

$$\sigma_a \propto \langle|a|\rangle, \qquad (2)$$

which holds when $\langle a\rangle=0$. (Note that this relation also holds for distributions other than a Gaussian.) More specifically, we estimate the noise by determining the absolute value of the stress at each lattice point of a slip plane (in our case on the $y=500$ plane). The absolute value of the stress is first averaged over the slip plane, then averaged over many simulations. We find that the average of that stress is zero and its distribution is essentially Gaussian, so the calculated quantity is proportional to the standard deviation of the stress distribution and thus is a measure of the fluctuations in the forces acting on a dislocation as it moves through the system. We refer to this quantity as $\mathcal{R}(t,N)(\propto\sigma_\sigma)$, or simply the "noise." An example is shown in Fig. 2, where we plot the noise versus the number of relaxation steps. Since the physi-

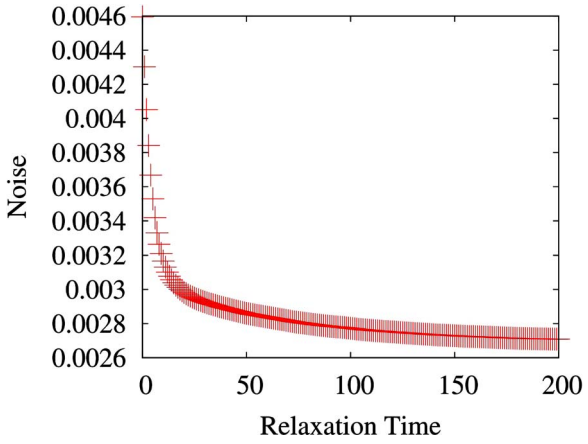

FIG. 2. (Color online) Plot of noise distribution, $\mathcal{R}(t,N=100)$, as a function of relaxation "time." The data are for 100 dislocations and averaged over 500 simulations.

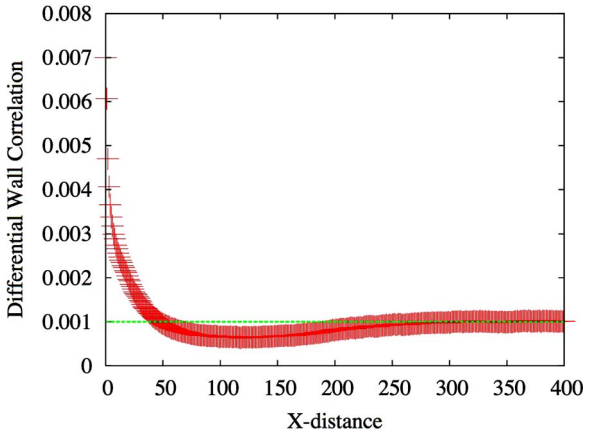

FIG. 3. (Color online) Plot of the function, $q(t=\infty,x,N=100)$ for $N=100$, showing a strong peak at the origin surrounded by a denuded region. The line at 0.001 corresponds to the correlation for a random distribution.

cal system relaxes with increasing time, which is analogous to the number of relaxation steps, for convenience we will refer to the number of relaxation steps simply as the time. $\mathcal{R}(t,N)$ is a function of both the relaxation time and the number of dislocations. The limited, partial, relaxation of $\mathcal{R}$ is a direct measure of the frustration frozen in the relaxed system, and will be employed to characterize the degree of that frustration.

The interaction energy of a reference dislocation in the presence of an infinite dislocation wall extending in the $\pm\hat{y}$ directions is[16]

$$E=\frac{\mu b^2}{4\pi(1-\nu)}\left\{\ln\{\cosh[2\pi(x-n)]-\cos(2\pi y)\}-\frac{2\pi(x-n)\sinh[2\pi(x-n)]}{\cosh[2\pi(x-n)]-\cos(2\pi y)}+\ln 2\right\}, \tag{3}$$

with x and y defined as before, and n is the index for a cell in the $\hat{x}$ direction. As for the force, the sum over n supercells in the $\hat{x}$ direction is extended to seven cells to the left and right of the central supercell. The log term is chosen to make the pair energy go to zero at infinite separation.[16]

The degree of order is derived from the standard pair correlation function for a configuration, $\mathcal{C}(t,x,y)$, which is the probability that a second dislocation will be found at x,y, given that the first dislocation is at $x,y=0$ at a relaxation time t.[7,8] There is a directional dependence to $\mathcal{C}$, so that $\mathcal{C}$ does not depend simply on the scalar distance to the field dislocation. We define the *differential* wall correlation function $q(t,x,N)$ as the sum of $\mathcal{C}$ over the direction vertical to the slip plane,

$$q(t,x,N)=\sum_y{}'\mathcal{C}(t,x,y). \tag{4}$$

The sum is over the lattice sites in the y direction, except the site at the reference dislocation, and $q(t,x,N)$ is normalized to the total number of dislocation pairs. According to this definition, $q(t,x,N)$ is a function of time, t the distance, x between the two members of a pair, and N. We will write $q(\infty,x,N)$ for the fully relaxed differential wall correlation function.

We now define an additional correlation function, $\xi_w(t,N)$, to serve as the basis for our analysis, which we will call the total wall correlation function, or just the wall correlation function. This function represents the total excess fraction of pairs that coagulate in a central wall as the system relaxes for a given value of N. That is, for a given N, the wall correlation function is defined as the sum over x of $q(t,x,N)$ for each relaxed state for which $q(x)>q(random)$, where $q(random)=1/L=0.001$ is the differential wall correlation function for a completely random distribution of dislocations (on a 1000×1000 lattice),

$$\xi_w(t,N)=\sum_{q(x)>q(random)}q(x). \tag{5}$$

This function, $\xi_w(t,N)$, is averaged over many simulations. As we shall see below (e.g., Fig. 3), when $q(t,x,N)$ is plotted as a function of x, there is a depleted region near the central peak, where $q(x)<q(random)$; the sum in Eq. (5) is only taken over the central peak to the left of the depleted region.

An additional variable of interest is the fractal dimension of the relaxed dislocation structure. However, since our results on the fractal character of the dislocation distribution only confirm reports by others,[17,14] those results are not displayed here.

III. SIMULATION RESULTS

A. The idea of an ensemble

A system of dislocations is an example of a classic "complex (mechanical) system." The question arises whether there are emergent properties of such a system that can be discerned. There has been a wide-spread faith that there are very few macroscopic variables that fully characterize the results of metallic deformation. Since the current system is a highly abstracted version of a deforming system, if emergent properties exist for the more complex physical system, such

emergent variables (hopefully the same ones) will be present here. We begin our search by defining an object that should exhibit these properties. That object is a *set* of simulations. This set of simulations has much of the character of an ensemble of states, such as defined in thermodynamics, except in our case, there is no temperature variable. Nevertheless, we will term the set of simulations an ensemble or macro system, since for each ensemble, one can define a set of macroscopic variables. These variables are the ones we have already used: the total number of dislocations in the simulation, the average interaction energy per dislocation as a function of the relaxation of the ensemble, the correlation functions, etc. The hope is that when the functional relationships between the various macrovariables have been laid out, some laws can be perceived between them that describe the overall (emergent) behavior of the system.

It is important to keep in mind that the defining property of all edge dislocation systems is the peculiar angular dependence of the force law. This angular behavior is crucial, because it frustrates the ability of the system to achieve a well-defined, ordered, ground state. The frustration, in itself, is difficult to characterize quantitatively, but is very closely associated with the average noise on the slip plane, what we have called $\mathcal{R}$.

It is also useful to keep in mind that we have simplified the dislocation system sufficiently that the change in energy in a simulation is closely connected with the vertical ordering of pairs. However the energy is also lowered when a shallow pair separates on the slip plane, so there are two independent ways to lower the energy. Our hope is that we can see how the part of the energy associated with vertical ordering is connected in a general way to the overall energy change in this relatively simple system.

B. Numerical results

In Fig. 2 we showed the relaxation with time of $\mathcal{R}(t,N=100)$, the noise parameter, in a simulation with $N=100$ dislocations. The relaxation shows a sharp initial (exponential) decrease, followed by a slow relaxation to its final value. A plot of the energy, calculated with Eq. (3), shows a similar behavior as it relaxes to its final value.

Figure 3 shows the (relaxed) differential wall correlation function, $q(t=\infty,x,N=100)$, for $N=100$ as a function of the distance from the reference wall. We note that for ten or less dislocations, there is a well pronounced sharp peak at the midpoint of the basic cell, corresponding to just two well developed "walls" 500 lattice spaces distant from one another. For more than ten dislocations, $q(x)$ loses the strong maximum at the midcell point. Hereinafter, we shall concentrate on the systems with $N>10$.

In Fig. 4 we show the variation of the noise, $\mathcal{R}(t,N)$, as a function of the number of dislocations for both the initial, random state ($t=0$) and the final, relaxed state ($t=\infty$). Note that both quantities follow a power law of the form $\mathcal{R}\propto N^{\alpha}$, with $\alpha=0.5686\pm.0120$ for the initial random configurations and 0.5042 ± 0.0122 for the relaxed states. Similarly, in Fig. 5 we show the variation of the relaxed wall correlation function, ξ_w, as a function of the number of dislocations. It too follows a power law with N, with an exponent given by $-0.3606\pm.0140$. While we do not show the results, we find that the energy is essentially linear with N, with a power-law exponent of 0.998 ± 0.001.

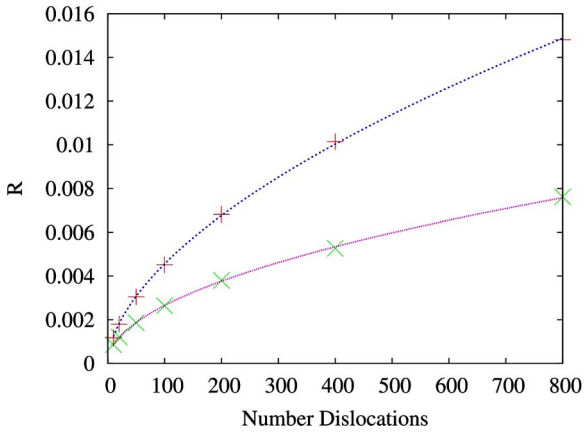

FIG. 4. (Color online) Initial $[\mathcal{R}(0,N)]$ and relaxed $[\mathcal{R}(\infty,N)]$ noise on the slip plane as a function of N. For the initial random state (upper curve), the power-law exponent is 0.5686 ± 0.0120 and for the final relaxed state (lower curve), the power is 0.5042 ± 0.0122.

It has often been assumed that the noise (in our case $\mathcal{R}$) scales as the square root of N (or ρ, the dislocation density).[3,12] We test that idea in Fig. 4 and indeed find that $\mathcal{R}$ has an exact (within the computed precision) square root dependence on N for the final relaxed configurations. There is a slight, but measurable, difference in the power exponent for the noise distribution found for the initial, random, configurations.

The important conclusion from the power law N dependence for the fully relaxed states is that all the fully relaxed ensemble variables are connected functionally as power laws to one another. For example, there is an inverse relationship between the wall correlation variable, $\xi_w(\infty,N)$, and the noise, $\mathcal{R}(\infty,N)$, for almost two orders of magnitude from $N=10$ to $N=800$,

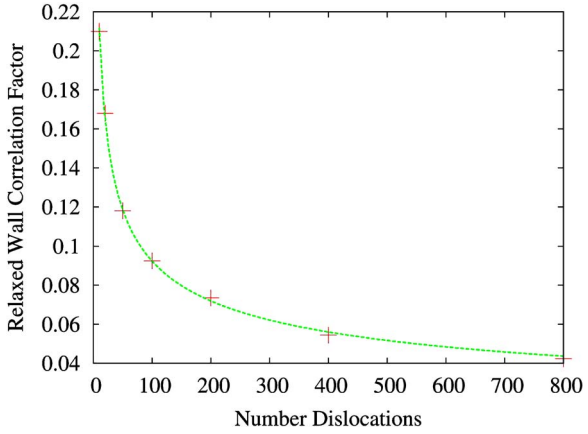

FIG. 5. (Color online) Relaxed wall correlation function $\xi_w(\infty,N)$. The exponent in the power law is -0.3606 ± 0.0140.

$$\xi_w(\infty,N) \propto \frac{1}{\mathcal{R}(\infty,N)^{.734}}. \tag{6}$$

This direct functional relation between $\xi_w(\infty,N)$ and $\mathcal{R}(\infty,N)$ is consistent with our central physical understanding that as the noise increases, the order decreases. A similar direct functional relation can be written between the interaction energy of the ensemble and the noise,

$$\boldsymbol{e}(\infty,N) \propto -\mathcal{R}(\infty,N)^{1.97}, \tag{7}$$

where $\boldsymbol{e}(t,N)$ is the interaction energy of the ensemble per dislocation as a function of time and N. This power relation is, within the computational precision, simply a quadratic function.

IV. SYSTEM DRIVING FORCE FOR ORDERED WALL FORMATION

Having determined the power laws for the ensemble variables, the basic physics of the dislocation ordering problem has been demonstrated, including the complementary roles played by the noise and energy. However, it is possible to take a significant step beyond this point, and to develop a conceptual framework for the formation of ordered structures in deformation and how that is related to the noise. We do this by introducing an *ensemble driving force* that governs the behavior of the macrovariables on their approach to the relaxed state, which is analogous to the thermodynamic force defined for thermodynamic systems.

The interaction energy of the macrostate per relaxed dislocation was defined earlier as $\boldsymbol{e}=\boldsymbol{e}(t,N)$, where the independent variables are the relaxation time and the number of dislocations in the system. For this system, t and N constitute a complete set of independent variables; if their values are known, the state of the ensemble is fully described. There are other configuration variables, however, such as $\xi_w(t,N)$ and $\mathcal{R}(t,N)$, that are also functions of the independent variables, $\{t,N\}$. The variation of the energy with respect to these other variables acts as an ensemble driving force on the system. Thus, a driving force for the formation of order for the system at fixed N can be defined as

$$\mathcal{F}_{\xi_w}(t,N) = -\left.\frac{\partial \boldsymbol{e}(t,N)/\partial t}{\partial \xi_w/\partial t}\right|_N, \tag{8}$$

where it is emphasized this is a derivative at fixed N.

A plot of $\mathcal{F}_{\xi_w}$ as a function of time (not shown) indicates that there is an initial fast exponential relaxation, followed by a much longer relaxation that follows a drastically different functional form. We define τ as the relaxation time of the initial fast exponential relaxation. 2τ corresponds to a relaxation of $\mathcal{F}_{\xi_w}$ to something like 90% of its change from the initial random state. τ is small (of the order of 10), reflecting the initial fast relaxation time. The τ point for $\mathcal{F}_{\xi_w}$ shows a small dependence on the number of dislocations N.

We will work with $\mathcal{F}_{\xi_w}$ in the very restricted region where $t \approx 2\tau$. The region of interest is limited for smaller t by the discreteness of the system and for larger t by the change of the functional form of the relaxation. In the vicinity of $t \approx 2\tau$, however, the system can be described by a well-defined analytic set of power laws and $\mathcal{F}_{\xi_w}$ can be computed from the fitted analytic exponential functions for $\boldsymbol{e}$ and ξ_w. We show $\mathcal{F}_{\xi_w}$ (at $t=2\tau$) as a function of N in Fig. 6.

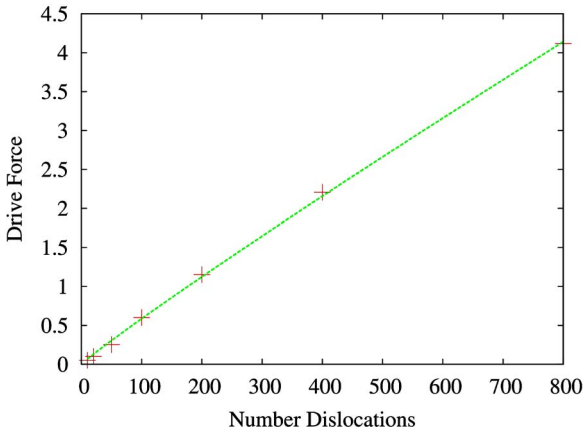

FIG. 6. (Color online) The driving force at $t=2\tau$ as a function of N, $\mathcal{F}_{\xi_w}(t=2\tau,N)$. The power exponent is 0.9411 ± 0.0480.

The noise term evaluated at $t=2\tau$, $\mathcal{R}(t=2\tau,N)$, displays the characteristic square root function between the noise and N (as in Fig. 4). Because both $\mathcal{F}_{\xi_w}(2\tau,N)$ and $\mathcal{R}(2\tau,N)$ are power functions of N, we can eliminate N and express the functional relation between them as

$$\mathcal{F}_{\xi_w} \propto \mathcal{R}^r$$

$$r=2. \tag{9}$$

This functional relationship between the driving force for order formation, and the resistance to order exerted by the noise is the primary result of the paper. This shows that at the relaxed equilibrium state, the energetic driving force is exactly in balance with the noise. At corresponding equilibrium states, the driving force is a quadratically increasing function of the noise. That is, as the noise increases, the driving force has to increase disproportionately to achieve the relaxed state. The exponent has the nominal value $r=2$ within the range of the computation precision.

If the ensemble force introduced here is to have the normal attributes of a thermodynamic force, then the same forces which have been defined at the relaxed state should also operate throughout relaxation. Indeed, we find that the magnitude of the resisting noise force relative to the positive energetic ordering force increases uniformly as one starts at the unrelaxed state, and approaches the relaxed state. That is, the relative size of the two forces is a measure of the "distance" one is from the equilibrium relaxed state. The detailed numerical results are not given for the sake of brevity.

V. CONCLUSIONS AND INTERPRETATION

We have demonstrated a simple linear relation between the ensemble driving force for order formation, $\mathcal{F}_{\xi_w}(t=2\tau,N)$, and the square of the noise, $\mathcal{R}(t=2\tau,N)$, showing explicitly the balance at the relaxed state between

the driving force for ordered wall formation and the frustration resistance, or noise. Beyond this central result, we find that the fully relaxed ensemble variables are all power functions of the number of dislocations (i.e., dislocation density) in the system. Consequently, the set of ensemble variables are thus expressible as direct power functions of each other.

Many studies of dislocations have demonstrated the self-similar character of the dislocation system,[18–21] and we believe this is a fundamental characteristic underlying dislocation behavior. Likewise, the idea of a system ensemble is generally applicable to all dislocation systems, in two as well as three dimensions. Further, we expect the concept of slip plane noise and the driving force for order to be generalizable to any of these systems. If these systems are all self-similar, then the driving force and noise will be power functions of N. We thus expect that at the relaxed state, there will be an invariant relation between the driving force for order and the noise resistance force. Of course, these statements for other systems than the one developed here are conjectures, but the general scale invariant character of all dislocation systems make the conjectures plausible and suggest that the findings reported here may relate to corresponding findings in more complicated cases. This conjecture amounts to the invocation of a universality property for dislocation systems that could be very powerful, if true.

A direct comparison of the findings of this paper to the results of the purely stochastic, and highly simplified, model of Hähner *et al.*[2,4] cannot be made. Nevertheless, in this study, we have certainly demonstrated the essential action of the energy in determining the final relaxed state of order and shown that noise is not enough to account for subscale dislocation structures.

Our idea of a macrostate of the system and its relation to the microstate realizations of the system has a parallel meaning to the concept of canonical ensembles in ordinary statistical mechanics. It is suggestive to equate the fluctuating back stress, which is the entity resisting the achievement of order in the deforming system, to a kind of pseudotemperature,[22] because it is the energy fluctuations caused by finite temperature that constrain an ordinary thermal transition. However, in the present case, the noise fluctuations do not constitute an independent variable in the problem, but are self-consistent with the evolving configuration. In the parlance of stochastic dynamics, the dislocation system has multiplicative noise (a function of the evolving variable) rather than the additive noise found in a thermally driven system. Nevertheless, our introduction of quasithermodynamic ideas for the dislocation system far from equilibrium should be viewed as being in the same tradition being developed by Liu[22,23] and others who explore the idea of a quasitemperature for nonequilibrium mechanical systems, and by Ngan[24] who has shown how to define a quasifree energy for the dislocation system. It is of interest to note that the results here are modified by the presence of a "real" temperature. For example, thermally induced climbs will make it possible to overcome noise barriers, and less energetic driving forces will be necessary to achieve a relaxed state.

We find that the large magnitude of the back stress noise generates enormous fluctuations in all aspects of the dislocation system. That is, the pair correlation function, energy, and structure of the equilibrium configuration all fluctuate wildly from one realization or simulation to another, so that in the three-dimensional case, it will be necessary to explore the statistics of three-dimensional simulations in much the same way we have done here for the two-dimensional case in order to achieve serious predictability. That requirement places a very serious barrier to achieving direct three-dimensional simulation of physical results, given the great difficulty of performing even a single three-dimensional simulation. This conclusion puts a major priority on the development of simpler theoretical techniques and models for three dimensions, such as methods for constructing valid coarse graining techniques, on the development of other two-dimensional models of deformation, and on the development of statistical models for the transport of strain through a system of assumed noisy three-dimensional patterns.

One approach to finding an approximate description of dislocation energetics in three dimensions has been to introduce a coarse-graining volume and to divide the problem into a long-ranged part (described with a multipole expansion) and a short-ranged, or local, part.[25–27] While the results to date are encouraging, especially with regard to the treatment of the long-ranged interactions, a major uncertainty has been the development of a method to predict the local, short-range order. While somewhat restricted in scope, we feel that the work reported here is an important first step in developing the correct phenomenology of ordering necessary to extend and refine the coarse-graining methods.

ACKNOWLEDGMENTS

The work of M. Koslowski and R. LeSar was performed under the auspices of the United States Department of Energy (US DOE under Contract No. W-7405-ENG-36) and was supported by the Division of Materials Science of the Office of Basic Energy Sciences of the Office of Science of the US DOE. MK thanks the Computational Materials Science Network of the US DOE/OS/OBES/DMS for their support.

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