Optimization and Plasticity in Disordered Media

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We study the plastic yielding of disordered media using the perfectly plastic random fuse model. The yield surfaces are shown to be different from those obtained minimizing the sum of the local yield thresholds, i.e., the so-called minimum ''energy'' surfaces. As a result, the global yield stress is lower than expected from naive optimization and the difference persists as the sample size increases. At variance with minimum energy surfaces, height-height fluctuations of yield surfaces exhibit multiscaling. We provide a theoretical argument that explains how this behavior arises from the very different nature of the optimization problem in both cases.

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When subject to large loads, materials can deform plastically, changing irreversibly their shape. Macroscopically, this process is described by the continuum theory of plasticity, stating that at the yield stress the sample develops plastic strain. There has been much interest in the so-called perfect plasticity (PP) limit, when plastic strain grows without any further increase of the external stress. In crystalline materials yielding is explained as the motion of dislocations in response to the applied stress [1]. In contrast, yielding in amorphous materials is due to irreversible atomic rearrangements. The latter has been mostly studied by means of extensive molecular dynamics simulations [2–5]. The insight gained through the numerics has led to mean field descriptions based on localized events in shear transformation zones (STZ) (see [2,6] and references therein).

Bridging gap between the length scales of microscopic models and continuum theories is yet one of the most challenging problems in materials science. The main difficulty for homogenization processes stems from the strong localization of plastic strain into slip lines—in crystals—or shear bands—in amorphous media. Nevertheless, some efforts have been made to study plastic deformations at mesoscopic scales [7–10]. In this framework, the yield surface results from the joint optimization of local intrinsic disorder and elasticity. The presence of local stress thresholds has been shown to induce the appearance of localization into shear bands.

Based on a powerful analogy, it is generally believed [10,11] that strain localization in the PP limit can be related to the problem of finding the minimum energy (ME) surface in a disordered medium. This is a generic optimization problem in disordered media in which one searches for the path that minimizes the sum of a given local random variable that is called ''energy.'' The conjectured equivalence between PP and ME comes from the observation that, at the yield point, it is not possible to find an elastic path, along which the stress could increase, spanning the sample from end to end [10,11]. In a disordered medium, the local yield stress σ_i of a given cross-section is in general a quenched random quantity. Therefore, according to Refs. [10,11], the global yield stress σ_c could be obtained by finding the surface $\mathcal{S}$ where the sum of the local yield stresses (the energy) is minimized (i.e., $\sigma_c = \min_{\mathcal{S}}[\sum_{i\in\mathcal{S}}\sigma_i]$). When this value of the stress is reached, the system would be divided into two disconnected elastic parts and would thus behave as perfectly plastic.

ME surfaces in disordered media have been intensively studied in the last 20 years since they appear in many contexts and several results are known exactly [12]. In particular, the ME surface in two dimensions is equivalent to a directed polymer at zero temperature and is thus a self-affine object with a roughness exponent $\zeta = 2/3$ and an energy exponent $\theta = 1/3$, describing the system size scaling of the energy fluctuations. The latter implies that yield stress for PP is expected to display finite-size corrections of the type $\sigma_c = \sigma_\infty + AL^{\theta-1}$. These corrections are particularly intriguing since they naturally connect to size effects that have recently been reported at micron scales both in crystals [13] and amorphous materials [14]. In particular, the case of metallic glasses is currently a fertile ground for research [14–18]. Microscopic and nanoscopic samples are known to display way bigger yield strengths and stresses than bulk samples from the same material but this size-dependence vanishes with sample diameters only tens of microns larger. This behavior surprisingly fits the kind of size scaling that ME interfaces display. Nonetheless, recent results using a shear plane yield criterion revealed size-independent properties at micron scales as well [17,19].

In this Letter we argue that the relation between PP and ME should be revised. By numerical simulations and theoretical arguments we show that PP and ME actually corre-

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spond to two different optimization problems in disordered media. As a consequence, the yield stress for PP is indeed smaller than the one observed for the equivalent ME problem, while the critical exponents of the surface and energy fluctuations appear to be the same. In two dimensions the yield surfaces have a roughness exponent of approximately $\zeta = 2/3$, and the yield stress fluctuations scale with an exponent close to the $\theta = 1/3$ that corresponds to the ME universality class. However, the specific surfaces are different in the two cases. Indeed, the geometry of the surface in the PP problem shows the presence of overhangs and large steps that lead to *multiscaling*—a dependence of the (qth order) roughness exponent on the order of the correlation function. The presence of overhangs has a significant effect on the global yield stress. Contrary to what happens in the common ME problems, overhangs lower the global yield stress so that a trivial minimization of the sum of local yield stresses is not accomplished.

In our numerical simulations we used the random fuse model (RFM) [20], which represents a scalar lattice electrical analog of the elasticity problem where the stress (σ), local elastic modulus (E), and strain (ϵ) are mapped to the current density (J), local conductance (g), and local potential drop (v), respectively. The usual procedure, widely applied to investigate quasibrittle materials, consists of fixing the fuse conductivities to unity, $g_i = 1$, and assigning to each fuse a random quenched threshold current T_i extracted from, e.g., a uniform distribution [21]. An external voltage (''strain'') is imposed between two bus bars placed at the top and the bottom of the system, and periodic boundary conditions are imposed in the horizontal direction. In studies of brittle fracture the fuses behave linearly until they fail irreversibly when the local current reaches its threshold $|J_i| \geq T_i$. However, we are interested here in the plastic response and thus the local current (local stress) remains constant and equal to the threshold $|J_i| = T_i$, regardless of the local voltage (strain).

The simulation of the plastic process consists of yield iterations. At each update, the Kirchhoff equations are solved to determine the local currents flowing in the lattice. We then increase the voltage up to the point where the most susceptible fuse yields. After each yield event, the new currents are computed using the tangent algorithm introduced by Hansen and Roux [10] and the process is iterated. After a large number of iterations, a yield surface is eventually formed across the sample. This is the PP yield surface in the sample, which is univocally determined for each disorder realization. On the other hand, the corresponding ME surface for the same disorder realization is calculated by using the Edmonds-Karp algorithm [22]. Note that, contrary to the brittle RFM, in the PP problem there are no avalanches. This is due to the fact that there is no current (stress) enhancement after yield events and thus stresses are not redistributed unlike in the brittle RFM and other models with avalanches [21].

For the RFM the need to solve a large system of linear equations for each update implies a high computational cost and limits the system size and the statistical sampling. While in the past the best performance was achieved by conjugate gradient methods [23], recently, a new algorithm [24,25] based on rank-1 downdate of sparse Cholesky factorizations has been introduced, which can largely reduce the computational cost of the simulations in the RFM. This has allowed to reach larger system sizes and improve sampling in smaller systems. Here we make use of this algorithm to study two-dimensional networks of fuses in diamond lattices. We study systems of linear size ranging from $L = 50$ to $L = 200$ and 10^4 realizations of the disorder.

Figure 1 (top panel) shows typical ME and PP yield surfaces for the same disorder configuration in a typical realization of the RFM. One can clearly see that the resulting interfaces may partially overlap but are clearly different. In particular, the PP surface presents very visible overhangs. As a consequence, the energy of the PP surface (which corresponds to the sum of thresholds over the yield path) is indeed higher than that for the ME surface. However, the actual current (yield stress) through the PP surface is lower than its energy, and also lower than that for the ME surface.

We claim that the difference between PP and ME surfaces for the *same* disorder realization can be explained by the following theoretical argument. The equivalent yield stress for the ME problem in a system of lateral size L is given by

$$\sigma_{c,\mathrm{ME}} = \sum_{i \in \mathcal{S}} T_i / L, \tag{1}$$

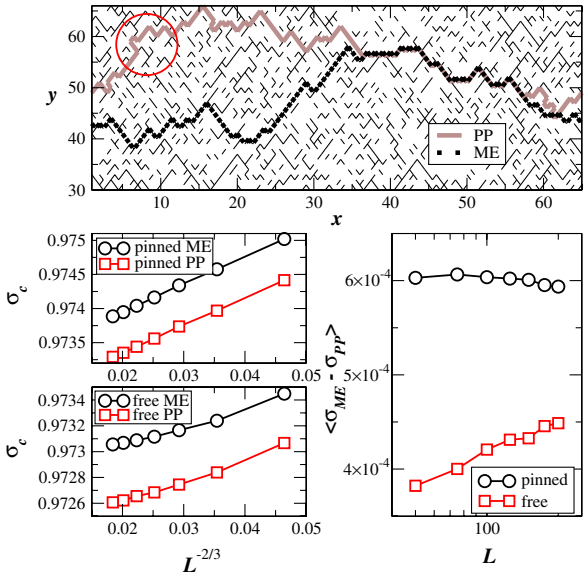

FIG. 1 (color online). Top: A typical ME and PP yield surface for the same disorder realization in a $L = 64$ diamond lattice. Bottom: On left panel, scaling of critical stress with system size in ME and PP for both, fixed and free ends. Right panel shows that the difference between the critical stress for ME and PP grows slowly but systematically or remains approximately constant with system size for free or pinned ends, respectively.

where i runs over all the bonds in the yield surface $\mathcal{S}$ that minimizes (1). In contrast, the PP surface $\mathcal{S}'$ would be the surface that requires a lowest external stress to appear and, therefore, the one that minimizes

$$\sigma_{c,\mathrm{PP}} = \sum_{i \in \mathcal{S}'} (\mathbf{n}_i \cdot \mathbf{j}_i) T_i / L, \tag{2}$$

where $\mathbf{n}_i$ is the unit vector locally normal to the surface at i, and $\mathbf{j}_i = \mathbf{J}_i/|J_i|$ is the local current flow direction. Equation (2) corresponds to the definition of the current flowing through an arbitrary surface.

If the surface had no overhangs we would have $\mathbf{n}_i \cdot \mathbf{j}_i = 1$ for all i and the same surface $\mathcal{S} = \mathcal{S}'$ would minimize both Eq. (1) and (2). However, in the presence of overhangs, it could happen that locally $\mathbf{n}_i \cdot \mathbf{j}_i = -1$ so that the surfaces $\mathcal{S}$ and $\mathcal{S}'$ are no longer the same. Indeed, we find that $\sigma_{c,\mathrm{PP}} < \sigma_{c,\mathrm{ME}}$, although the sum of thresholds along the PP path is naturally higher than $\sigma_{c,\mathrm{ME}}$. Therefore, the mapping between minimum energy and yield stress exists only for fully directed surfaces ($\mathbf{n}_i \cdot \mathbf{j}_i = 1$ for all i), where the total yield stress can be calculated as the sum of local yield stresses. Physically, this means that PP and ME actually correspond to two different optimization problems. A PP path may find it very advantageous to develop overhangs in order to minimize Eq. (2) due to the negative contributions coming from the $\mathbf{n}_i \cdot \mathbf{j}_i < 0$ terms. On the contrary, for the ME surface one has to minimize (1) and overhangs generally increase the global energy and are thus normally avoided, unless disorder has a very broad distribution [26].

The difference between the ME and PP yield stresses is quantified in Fig. 1. Two different boundary conditions have been studied: the two ends of the path are either left free or pinned at midsystem. These two situations correspond to finding either a global or local minimal surface, respectively. Left panel shows the yield stress scaling with system size for both free and fixed boundary conditions. In both cases the existence of a finite-size correction becomes apparent, as well as the fact that $\sigma_{c,\mathrm{PP}}(L) < \sigma_{c,\mathrm{ME}}(L)$ is always satisfied. For fixed boundary conditions we find $\sigma_c = \sigma_\infty + AL^{-2/3}$ leading to $\theta = 1/3$, which is the expected result for the ME universality class and likewise so for the PP problem. Right panel shows the average yield strength difference $\langle \sigma_{c,\mathrm{ME}} - \sigma_{c,\mathrm{PP}} \rangle$ that systematically increases with L for free boundary conditions or remains constant in the case of fixed boundary conditions.

The scaling of the yield stress is reminiscent of size effects, traditionally studied in brittle fracture problems, where one expects extreme value statistics to apply [27,28]. Although size effects and stress fluctuations have been recorded in microplasticity [13,14], it is not clear if they have the same origin as in fracture. Here, we measure the yield stress distribution for the PP and ME models. Figure 2 shows the rescaled yield stress cumulative distributions for both ME and PP problems with free and pinned boundary conditions. The latter corresponds to the usual ME problem studied in the literature while the "free" case

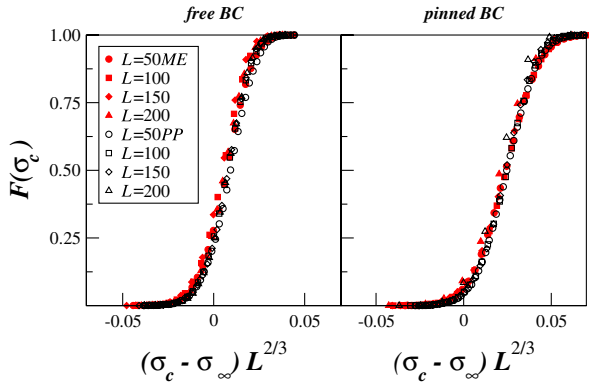

FIG. 2 (color online). Cumulative distributions of yield stress for free and pinned boundary conditions for ME and PP. The distributions can all be collapsed with the same exponent, related to $\theta = 1/3$.

is closer to experimental reality. We see that for both boundary conditions the distributions for PP and ME collapse with the same exponent into a very similar scaling function. Since for the ME problem with pinned boundary conditions we know that asymptotically the scaling function should converge to the Tracy-Widom distribution [29], we can speculate that this is also true for PP. We have also checked that Weibull and other extremal distributions are not appropriate to fit the data.

The spatial properties of the yield surfaces are analyzed in Fig. 3, where we show the qth order correlation functions, $C_q(\ell) = \langle |h(x+\ell) - h(x)|^q \rangle \sim \ell^{q\zeta_q}$, for PP and ME surfaces. A univaluated height is constructed by taking the maximum surface value $h(x)$ at each site x. ME surfaces exhibit the expected "simple" self-affine scaling, that is, the correlation function scales with the same roughness exponent $\zeta_q^{\mathrm{ME}} = \zeta^{\mathrm{ME}} = 2/3$ for all q. This is in agreement with previous studies showing that overhangs are irrelevant in ME surfaces below the strong disorder limit [26,30]. In

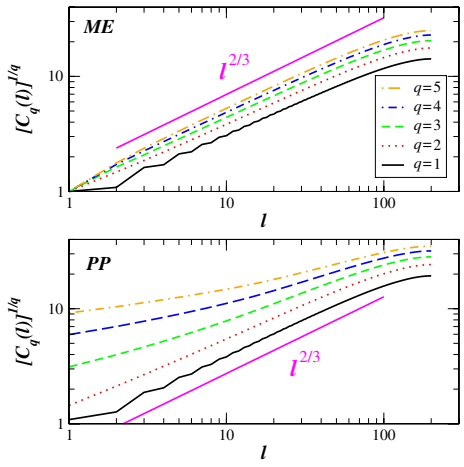

FIG. 3 (color online). Height-height correlation function of order $q = 1$ to $q = 5$ for ME and PP problems in a system of size $L = 200$. Multiscaling of the surface fluctuations for PP is clearly observed.

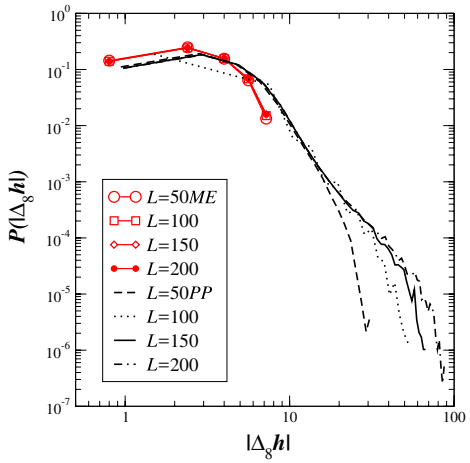

FIG. 4 (color online). Distribution of height differences at a fixed distance $\ell = 8$ in PP and ME for different system sizes. For PP the tail of the distribution grows with system size, while it remains constant for ME surfaces.

contrast, PP surfaces show strong deviations from simple self-affinity and the existence of multiscaling becomes readily evident in Fig. 3 (bottom panel). This indicates that overhangs are indeed relevant in PP surfaces. This is illustrated by studying the distribution of height differences at different length scales $\mathcal{P}(|\Delta_\ell h|)$ with $\Delta_\ell h \equiv h(x+\ell) - h(x)$. For a self-affine interface with roughness exponent α, this distribution is expected to scale as $\mathcal{P}(|\Delta_\ell h|) \sim \ell^{-\alpha} f(|\Delta_\ell h|/\ell^{-\alpha})$. To obtain further insight on the role of overhangs at different scales we analyze the distribution for intermediate values of $\ell \ll L$. In Fig. 4 it is shown that for ME surfaces $\mathcal{P}(|\Delta_8 h|)$ is narrow and independent of L, whereas for the PP surfaces the tail grows with L and approaches asymptotically a power-law shape, $\mathcal{P}(|\Delta_8 h|) \sim |\Delta_8 h|^{-2}$.

In summary, we have shown that the principle of load-sharing in a yielding material introduces the ''yield surfaces'' as a separate statistical mechanics problem. Our main result is that ME and PP correspond to two different optimization problems in disordered media. The reason for the nonequivalence between ME and PP surfaces arises from the fact that an actual yield surface—with signed currents—is created in a yielding material before the ME surface. This is intimately related to the peculiar properties of PP surfaces such as relevant overhangs, large height-height fluctuations, and lack of simple self-affinity. In addition, the yield stress displays a finite-size scaling form with corrections due to the boundary conditions. It would be interesting to study numerically more realistic models of plasticity, and to investigate the role of dimensionality since in three dimensions the large surface fluctuations are theoretically expected to diminish.

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