Power laws distributions as a signature of complexity: models from materials science

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Scale invariant power law distributions are ubiquitous to a wide variety of physical, chemical and biological systems ranging from geological to nanometer scales. Despite attempts by best of minds, the origin of power law distributions has remained mysterious. While we will not attempt to solve the general problem, we discuss three different physical situations drawn from materials science where power law distributions are reported. We show that models designed to capture the basic experimental features of the three physical situations automatically predict power law distributions. The three phenomena are the martensitic transformation (elastic), dynamics of peeling of an adhesive tape (visco-elastic) and the Portevin-Le Chatelier effect (plastic).

We first consider a two dimensional model for athermal martensite transformation. The model includes long-range interaction between transformed domains, inertial effects and dissipation that accounts for acoustic energy. The model predicts experimental features such as thermal hysteresis and, growth and shrinkage of martensite domains under thermal cycling. The model also predicts the power law distribution for the amplitude of the acoustic emission signals during thermal cycling seen in experiments [1].

We next consider the peel front dynamics of an adhesive tape pulled at a uniform speed. The model predicts broad features of the peel dynamics such as the stick-slip motion and the stuck-peeled configurations of the peel front. The model also predicts the power law distribution of acoustic energy reported in experiments.

The third example we consider is the Portevin-Le Chatelier (PLC) effect, a kind of instability found when metallic alloys are deformed in window of strain rates. Three types of bands and the associated serrations are found with increasing strain rate. Analysis of experimental stress signals corresponding to type A serrations show that the stress drop magnitudes follow a power law distribution. Again, the Ananthakrishna model designed to recover the generic experimental features of the PLC effect also captures the power law distribution for stress drop magnitudes.

In all these cases, the power law distributions emerge automatically once attempts are made to capture the generic features of the phenomenon. Surprisingly, in each of these cases, the power law distribution emerges purely from deterministic dynamics.

Portevin - LeChatelier like phenomena in confined compression of snow

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Snow is a cohesive-granular material of high porosity which is typically encountered at high homologous temperatures ( > 95% of its melting temperature). Thus, thermodynamically driven microstructure evolution - in particular sintering processes - may occur on the typical timescale of deformation experiments. Shear deformation of snow is associated with strain softening due to the breaking of necks connecting ice granules, but this softening may be counter-acted by age hardening associated with rapid sintering processes which lead to the formation of new necks/bonds. If both competing processes occur on a comparable time scale, complex spatio-temporal deformation patterns may be encountered in the form of stress oscillations and propagating deformation bands.

We present results of confined compression experiments which show such phenomena in the form of compaction bands which during the course of an experiment repeatedly propagate along the compression direction of a laterally confined snow sample. These bands are associated with oscillations in the measured stress strain curve which superimpose on a global hardening trend. The overall phenomenology presents strong analogies with the Portevin-le Chatelier phenomenon encountered in metal alloys in the temperature/strain rate regime where age hardening due to dislocation pinning by moving solutes occurs on a comparable time scale as strain-driven softening due to dislocations breaking free from solute clouds under the action of applied stress.

We formulate a theoretical model which generalizes established frameworks for solid foam plasticity to account for internal length scales associated with the snow microstructure, strain softening processes, and age hardening due to rapid sintering. We demonstrate that by considering typical materials parameters for snow this framework allows to fully reproduce the observed phenomena.
Dislocation Pattern Evolution and Strain Hardening in FCC Metals through Discrete Dislocation Dynamics Simulations

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Strain hardening in crystals and the accompanying dislocation pattern evolution (in the form of cell-like structures) are among the most difficult self-organizing behaviors to predict and explain. Screw character dislocation cross-slip has been typically presumed to play the main role in dislocation cell structure formation. However, many open questions remain regarding this mechanism. Recent molecular dynamics simulations showed that two cross-slip mechanisms, namely, surface and intersection mediated cross-slip mechanisms, exhibit a considerably lower activation energy than the traditionally accepted Friedel-Escaig cross-slip mechanism. In this work, we present the results of implementing these newly identified cross-slip mechanisms into discrete dislocation dynamics (DDD) simulations of nickel microcrystals, ranging in size from 0.5 to 10 microns in diameter. The conditions for each mechanism are discussed, along with their statistics and frequencies. The results show that dislocation cell structures form in simulation cells having diameters greater than 5 microns, as the dislocation density increases with increasing plastic strain. Smaller simulations cells however do not show any considerable cell formation at small strains as compared to the larger cells. These findings agree with recent experimental observations at the same crystal sizes.
Quantification and Comparison of Random Structures

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Random structures abound at all length scales in materials science. This includes the contact graph of atoms in a metallic glass and the covalent bonds in a chalcogenide glass at the atomic scale, and dense dislocation networks and the bonding of cross-linked polymers at the nanometer scale. Examples at the micrometer scale include the structure of aerogels and the grain boundary network of a polycrystal, and at the macro scale the packing of granular materials and the branching pattern of a tree.

One feature of all of these random structures is that they defy characterization by the usual approach used in crystallography, that is, by the identification of a periodic unit and the classification of defects as deviations from periodicity. Nevertheless, some means of characterization is clearly necessary. How else would one identify the changes in atomic disorder when annealing a metallic glass, or the changes in a dislocation network resulting from the activation of cross-slip? While previous researchers have proposed a variety of techniques, any given one is usually applicable to only a few of the above examples, and none of them is able to completely characterize the connectivity of a generic random structure.

Our approach is to map a small portion of the structure to a colored graph, known as a swatch, that gives a complete description of the local connectivity. By considering the probability distribution of swatch types, or local environments, we provide a complete characterization of the connectivity of the structure. That is, any question that may be asked about the connectivity may be answered using only this information. Furthermore, our classification admits a natural metric on the space of random structures. This allows us to, e.g., rigorously quantify the difference in the bonding of a metallic glass from a crystalline solid, or even to meaningfully compare the connectivity of a dislocation network and an aerogel. Finally, we provide evidence that these proposed quantities are practically computable.

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Spatiotemporal correlations between plastic events in the shear flow of amorphous solids: from molecular dynamics to mesoscopic models

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The slow flow of amorphous solids exhibits striking heterogeneities: swift localised particle rearrangements take place in the midst of a more or less homogeneously deforming medium. Correlations and interactions between plastic events that involve of order 25 particles (in 2D) control the evolution of the strain field on much longer length and time scales. Here we develop a mesoscopic (coarse-grained) model of plastic flow that is systematically linked to atomistic molecular dynamics simulations. We first determine the time-dependent elastic response of an amorphous medium to an isolated plastic event and show that, despite large fluctuations, it can be modeled with the picture of 2D Eshelby inclusions with an elastic Green’s function displaying quadrupolar symmetry, viz. $G(r) \sim \cos(4\theta)/r^2$ [1]. We then determine the full spatiotemporal correlation functions $C(\mathbf{r},t)$ (inset of figure for one value of $t>0$) between elementary plastic events in a sheared athermal glassy solid (main figure, color scale indicates level of nonaffine strain) [2]. Our mesoscopic description builds upon the picture of localized, short-lived and highly dissipative events observed in the MD simulations by considering elastoplastic blocks of size of a rearranging region. Upon reaching a local yield stress drawn from a disorder distribution, elastic interactions occur instantaneously and the local stress evolves according to

$$\dot{\sigma}(\mathbf{r}) = \mu \dot{\epsilon} + 2\mu \int d\mathbf{r} G(\mathbf{r},\mathbf{r}')\epsilon_{\text{pl}}(\mathbf{r}')$$

We achieve excellent agreement for all aspects of bulk rheology between atomistic simulations and this class of mesoscopic models. Quadrupolar plastic correlations (see figure) are also successfully reproduced, but quantitative agreement of dynamical plastic correlations requires considering additional physics, in particular including the effect of elastic heterogeneity on the propagation of shear waves as well as their finite propagation speed.

Spatial structure and time evolution of breaking bursts in a fiber bundle model of disordered materials

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The fracture of heterogeneous materials proceeds in bursts which can be recorded by optical, acoustic or electromagnetic techniques. Although crackling noise is the major source of information about the microscopic dynamics of fracture, its analysis mainly focuses on the statistics of crackling events considering fracture as a stochastic point-process. Here we investigate the temporal and spatial evolution of single bursts emerging in heterogeneous materials under a constant external load using a fiber bundle model. In the model fibers break due to two physical mechanisms: (i) a fiber breaks immediately when the load on it exceeds the local failure strength; (ii) fibers subject to load undergo an aging process accumulating internal damage and break when their damage exceeds a random threshold value. As a consequence under a constant load slowly damaging fibers trigger bursts of immediate breakings analogous to crackling avalanches in real experiments [1,2].

Computer simulations revealed a complex time evolution and spatial structure of single crackling bursts in the model (see Fig. 1 for an example). We demonstrate that when the stress redistribution after fiber failures is localized, the average temporal shape of crackling pulses has a right handed asymmetry due to the gradual acceleration of bursts. For long range interaction, however, a symmetric shape with parabolic functional form is obtained. In spite of the compact space-filling internal structure of bursts (Fig. 1), their external frontier proved to be a fractal with dimension $D_f = 1.25$. The same fractal dimension characterizes the geometrical structure of the propagating crack front along which bursts are localized. Our analysis revealed that the pulse shape and spatial evolution of bursts are correlated which can be exploited in materials testing [2].

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Field Dislocation Mechanics in the tectonic and sub-inter-supersonic regimes

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We explore the potential of modeling both sub-inter-supersonic dislocation motion and dynamic ruptures using Field Dislocation Mechanics (FDM), a non-linear, partial differential equation (PDE) based model of the mechanics of dislocations. A simplified two dimensional FDM model is developed and numerically studied. The model assumes the whole body to be elastic except for a thin layer governed by dislocation plasticity. Dislocations are assumed to move along the layer only. When modeling a fault, the layer is assumed to be elastically weaker than the surrounding and to admit elastic damage on the passage of the rupture front.

One of the main results is that FDM is demonstrated to be able to capture the kinetic relationship of a single dislocation in different velocity regimes (from subsonic to supersonic); qualitative agreement with a Molecular Dynamics simulation of a similar problem is obtained.

The 2-D model is then explored more to show some basic advancements of modeling tectonic phenomenon using FDM. The slip evolution at a spatial point due to the passage of a rupture front is found to be in agreement with short-slip-duration seismological observations. The traction profile shows a strong strengthening effect behind the rupture front as well. A transverse displacement field in qualitative agreement with observations from an earthquake is also shown. These results suggest that FDM is able to address some fundamental issues in dynamic rupture, making it a valuable complementary tool to conventional crack-mechanics based rupture models for the investigation of earthquake related phenomena.
After critically reviewing the early work on plastic instabilities – to which Ladislas Kubin was a major contributor (improving, among other things, the initial models by the author and coworkers on dislocation patterning, persistent slip bands, and Portevin-Le Chatelier bands) – the discussion is focused at the nanoscale. Example problems on size effects, intermittent plasticity and serrated flow are discussed. These require the incorporation of stochasticity in the previously advanced gradient plasticity models. It is also shown that interpretation of related statistical deformation features through usual power laws based on Boltzmann-Gibbs entropy do not hold and one needs to use Tsallis q-entropy considerations for modeling the experimental observations.