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Scaling theory of continuum dislocation dynamics in three dimensions: Self-organized fractal pattern formation

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ABSTRACT

We focus on mesoscopic dislocation patterning via a continuum dislocation dynamics theory (CDD) in three dimensions (3D). We study three distinct physically motivated dynamics which consistently lead to fractal formation in 3D with rather similar morphologies, and therefore we suggest that this is a general feature of the 3D collective behavior of geometrically necessary dislocation (GND) ensembles. The striking self-similar features are measured in terms of correlation functions of physical observables, such as the GND density, the plastic distortion, and the crystalline orientation. Remarkably, all these correlation functions exhibit spatial power-law behaviors, sharing a single underlying universal critical exponent for each type of dynamics.

1. Introduction

Dislocations in plastically deformed crystals, driven by their long-range interactions, collectively evolve into complex heterogeneous structures where dislocation-rich cell walls or boundaries surround dislocation-depleted cell interiors. These have been observed both in single crystals (Kawasaki and Takeuchi, 1980; Mughrabi et al., 1986; Schwink, 1992) and polycrystals (Ungár et al., 1986) using transmission electron microscopy (TEM). The mesoscopic cellular structures have been recognized as scale-free patterns through fractal analysis of TEM micrographs (Gil Sevillano et al., 1991; Gil Sevillano, 1993; Hähner et al., 1998; Zaiser et al., 1999), Fig. 1(a). The complex collective behavior of dislocations has been a challenge for understanding the underlying physical mechanisms responsible for the development of emergent dislocation morphologies.

Complex dislocation microstructures, as an emergent mesoscale phenomenon, have been previously modeled using various theoretical and numerical approaches (Ananthakrishna, 2007). Discrete dislocation dynamics (DDD) models have provided insights into the dislocation pattern formations: parallel edge dislocations in a two-dimensional system evolve into ‘matrix structures’ during single slip (Bakó et al., 1999), and ‘fractal and cell structures’ during multiple slip (Bakó et al., 2007; Bakó et al., 2007); random dislocations in a three-dimensional system self-organize themselves into microstructures through junction formation, cross-slip, and short-range interactions (Madec et al., 2002; Gomez-Garcia et al., 2006). However, DDD simulations are limited by the computational challenges on the relevant scales of length and strain. Beyond these micro-scale descriptions, CDD has also been used to study complex dislocation structures. Simplified reaction–diffusion models have described persistent slip bands (Walgraef and Aifantis, 1985), dislocation cellular structures during multiple

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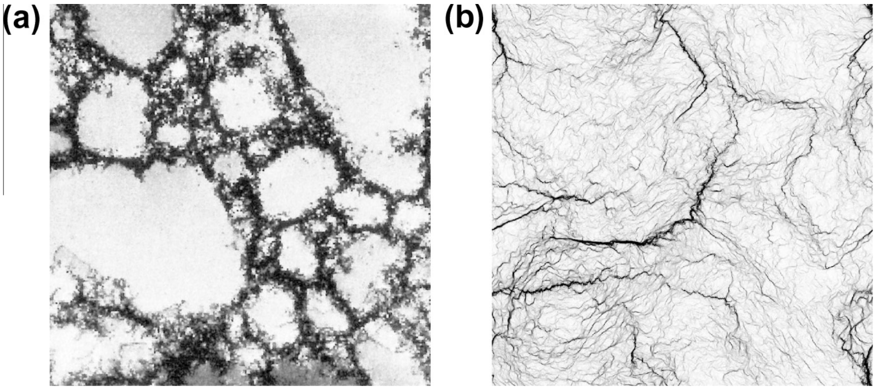

Fig. 1. Experimental and simulated dislocation cellular structures. In (a), a typical TEM micrograph at a micron scale is taken from a Cu single crystal after [1 0 0] tensile deformation to a stress of 76.5 MPa (Hähner et al., 1998); in (b), a simulated GND density plot is shown. Note the striking morphological similarity between theory and experiment.

slip (Hähner, 1996), and dislocation vein structures (Saxlová et al., 1997). Stochasticity in CDD models (Hähner et al., 1998; Bakó et al., 1999; Groma and Bakó, 2000) or in the splittings and rotations of the macroscopic cells (Pantleon, 1996; Pantleon, 1998; Sethna et al., 2003) have been suggested as an explanation for the formation of organized dislocation structures. The source of the noise in these stochastic theories is derived from either extrinsic disorder or short-length-scale fluctuations.

In a recent manuscript (Chen et al., 2010), we analyzed the behavior of a grossly simplified continuum dislocation model for plasticity (Acharya, 2001; Roy and Acharya, 2005; Acharya and Roy, 2006; Limkumnerd and Sethna, 2006; Chen et al., 2010) – a physicist's 'spherical cow' approximation designed to explore the minimal ingredients necessary to explain key features of the dynamics of deformation. Our simplified model ignores many features known to be important for cell boundary morphology and evolution, including slip systems and crystalline anisotropy, dislocation nucleation, lock formation and entanglement, line tension, geometrically unnecessary forest dislocations, etc. However, our model does encompass a realistic order parameter field (the Nye-Kröner dislocation density tensor (Nye, 1953; Kröner, 1958) embodying the GNDs), which allows detailed comparisons of local rotations and deformations, stress, and strain. It is not a realistic model of a real material, but it is a model material with a physically sensible evolution law. Given these simplifications, our model exhibited a surprisingly realistic evolution of cellular structures (Fig. 1(b)). We analyzed these structures in two-dimensional simulations (full three-dimensional rotations and deformations, but uniform along the z-axis) using both the fractal box counting method (Gil Sevillano et al., 1991; Gil Sevillano, 1993; Hähner et al., 1998; Zaiser et al., 1999) and the single-length-scale scaling methods (Hughes et al., 1997; Hughes et al., 1998; Mika and Dawson, 1999; Hughes and Hansen, 2001) used in previous theoretical analyses of experimental data. Our model qualitatively reproduced the self-similar, fractal patterns found in the former, and the scaling behavior of the cell sizes and misorientations under strain found in the latter (power-law refinement of the cell sizes, power-law increases in misorientations, and scaling collapses of the distributions).

There are many features of real materials which are not explained by our model. We do not observe distinctions between 'geometrically necessary' and 'incidental' boundaries, which appear experimentally to scale in different ways. The fractal scaling observed in our model may well be cut off or modified by entanglement, slip-system physics, quantization of Burgers vector (Kuhlmann-Wilsdorf, 1985) or anisotropy – we cannot predict that real materials should have fractal cellular structures; we only observe that our model material does so naturally. Our spherically symmetric model obviously cannot reproduce the dependence of morphological evolution on the axis of applied strain (and hence the number of activated slip systems); indeed, the fractal patterns observed in some experiments (Hähner et al., 1998; Zaiser et al., 1999) could be associated with the high-symmetry geometry they studied (Wert et al., 2007; Hansen et al., 2011). While many realistic features of materials that we ignore may be important for cell-structure formation and evolution, our model gives clear evidence that these features are not essential to the formation of cellular structures when crystals undergo plastic deformation.

In this longer manuscript, we provide an in-depth analysis of three plasticity models. We show how they (and more traditional models) can be derived from the structures of the broken symmetries and order parameters. We extend our simulations to 3D, where the behavior is qualitatively similar with a few important changes. Here we focus our attention on relaxation (rather than strain), and on correlation functions (rather than fractal box counting or cell sizes and misorientations).

Studying simplified 'spherical cow' models such as ours is justified if they capture some key phenomenon, providing a perspective or explanation for the emergent behavior. Under some circumstances, these simplified models can capture the long-wavelength behavior precisely – the model is said to be in the same universality class as the observed behavior (Sethna, 2006, Chapter 12). The Ising model for magnetism, two-fluid criticality, and order–disorder transitions; self-organized critical models for magnetic Barkhausen noise (Sethna et al., 2001; Durin and Zapperi, 2006) and dislocation avalanches (Zaiser, 2006) all exhibit the same type of emergent scale-invariant behavior as observed in some experimental cellular structures (Hähner et al., 1998). For all of these systems, 'spherical cow' models provide quantitative experimental predictions of