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Folding in metal polycrystals: Microstructural origins and mechanics

Narayan K. Sundaram [a, *], Anirban Mahato [b], Yang Guo [c], Koushik Viswanathan [d], Srinivasan Chandrasekar [d]

[a] Department of Civil Engineering, Indian Institute of Science, Bangalore, 560012, India
[b] Department of Mechanical Engineering, Indian Institute of Technology, Patna, 801103, India
[c] Department of Mechanical Engineering, Michigan State University, East Lansing, MI, 48823, USA
[d] Center for Materials Processing and Tribology, Purdue University, West Lafayette, IN, 47907, USA

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ABSTRACT

Surface folding in large-strain deformation of metal polycrystals, mediated by unsteady sinuous plastic flow, was recently uncovered by direct observations. Here, we examine microstructural origins and mechanics of the folding process in polycrystalline aggregates, using computational methods and *in situ*, high-speed imaging experiments. Our model loading system is an indenter contact that imposes large strain deformation typical of metal forming, sliding and cutting.

Folding arises primarily from intrinsic, grain-level flow stress variation in the polycrystalline ensemble. This flow stress heterogeneity is incorporated, spatially, in a continuum Lagrangian finite element framework, by partitioning the metal surface into grain-like structures. This pseudograin model captures all key aspects of the folding as observed by direct imaging, from fold nucleation via microstructure heterogeneity through various stages of fold development on the surface; surface strain fields; and deformation parameter effects such as indenter geometry and friction. The folding phenomenon is quite general, and provides a direct route for formation of surface defects and delamination wear particles. The microstructure-based simulation capability, thus validated, can be used as a virtual tool for analyzing large-strain plastic flow at surfaces and its consequences. Besides demonstrating the importance of folding in surface plasticity, the study points to a critical need to consider microstructure effects on local plasticity for sliding wear and deformation processing.

1. Introduction

Plastic flow at metal interfaces is a central feature of phenomena and processes as diverse as friction in metals [1,2], sliding wear [3–5], machining [6,7], deformation processing [7–9], and indentation [10–13].

The systems involved in interfacial plasticity are characterized by a hard tool or indenter in contact with, and in relative motion to, a softer substrate or workpiece, with large accompanying plastic strains. A historically well-studied system of this kind is a hard wedge sliding against a metal, representative of the interaction of a single asperity with a substrate in sliding wear and abrasive cutting [14,15], and die/tool workpiece contacts in manufacturing processes. Recent *in situ* imaging experiments have shown that this apparently simple system is capable of exhibiting very complex, unsteady plastic flow patterns even at room temperature and at low speeds. These flow patterns include surface fold (self-contact) formation in sliding [16] and highly sinuous flow in cutting of annealed metals [17]. These patterns have also been sought at the sub-micron scale using molecular dynamics simulations [18].

It is now known that these complex flow patterns have important engineering consequences. For instance, direct imaging reveals that surface folds[1] that form on the prow ahead of a sliding indenter become crack-like features after passing the tip of the indenter. These crack-like features have adverse consequences for wear and surface quality [19]. Moreover, folding can impose severe constraints on the use of sliding-type processes for the generation of surfaces with fine-grained microstructures and graded properties. This necessitates careful selection of processing conditions to achieve a desired surface quality [20]. Thus, in addition to its

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* Corresponding author.
E-mail address: nsundaram@civil.iisc.ernet.in (N.K. Sundaram).

[1] We define folds as surface features arising from self-contact, and do not use the term 'fold' in the more loose sense of inhomogeneous surface deformation.

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importance as a mode of inhomogeneous deformation in metal plasticity, folding is quite relevant to materials manufacturing and wear.

Prior work [16] has revealed conditions under which plastic flow patterns like folding and sinuous flow develop in simple sliding systems. The first condition is a free surface neighboring the contact, which greatly expands the kinematic possibilities. Secondly, folding has been observed at the mesoscale ($100\ \mu$m-$2000\ \mu$m) implying an obvious length-scale effect. It was conjectured by us in Ref. [16] that a parameter η, defined as the ratio of the grain size to a characteristic plastic zone size, plays a key role in fold formation. The third requirement is ductility, without which failure occurs rather than folding.

However, these conditions are hardly restrictive, and a key motivating factor for the present work is to establish that folding is an important and heavily microstructure-controlled pattern of plastic flow, with concomitant surface damage. A secondary motivating factor is to address some important open questions in the mechanics of folding, particularly the role of material microstructure and deformation parameters such as geometry and interfacial friction.

The present work is a comprehensive computational (finite element) and experimental investigation of folding in a representative metal polycrystal (Al-1100), under conditions typical of sliding contacts and surface deformation processing. We show that folding is a quite general plasticity phenomenon under these loading conditions. We do this in the framework of a plane strain sliding contact between a hard wedge and a metal workpiece. Folding is shown to provide a direct avenue for formation of wear particles by delamination, and surface defects like cracks and tears. Microstructure-related flow stress heterogeneity, which is critical for the nucleation and development of folds [16], is incorporated in a simple but highly effective finite element model.

2. Finite element simulation procedure

2.1. Pseudograin model and mesh partitioning for polycrystals

At the experimental length scales of interest, the metal workpiece must be treated as a (spatially inhomogeneous) polycrystalline aggregate. Depending on the value of the parameter η one has a few to a few dozen grains[2] in the deformation zone. To this end, a simplified or ‘pseudograin’ model is used to introduce spatial heterogeneity in the plastic flow properties. The idea is to partition the mesh into a set of pseudograins,[3] and assign different flow properties to each grain so as to achieve a desired mean hardness value for the specimen. Grain boundaries are idealized as perfect, and topological constraints on the grain morphology are not explicitly enforced. For simplicity, the elastic response of individual pseudograins is modeled as isotropic. The pseudograin approach echoes the elementary principle of polycrystalline plasticity that slip initiates more easily in some grains than others based on the critical resolved shear stress τ_{CRSS}.

A portion of a typical planar FE mesh used for the sliding analyses is shown in Fig. 1. The mesh is structured so as to have a high element density in a fine-meshed, near-surface region about $550\ \mu$m deep. A mesh fanning algorithm is used to rapidly increase element size away from this region. After generation, the mesh is partitioned into grains in three steps. First, polygonal pseudograins of a specified mean size D_0 are obtained using a Voronoi approach, commonly employed in crystal plasticity finite element (CPFE) simulations [21]. This is done by generating a point-set $\boldsymbol{P} = \boldsymbol{x}_k$ in a plane region. The separation between these points is random, but distributed about a specified mean. The Voronoi diagram of this set of points is then found, yielding a set of convex polygons. The interior of the kth Voronoi polygon $\mathbb{C}_k$ is given by Ref. [22]

$$\mathbb{C}_k = \left\{ \boldsymbol{x} \in \mathbb{R}^2 : \left\| \boldsymbol{x} - \boldsymbol{x_k} \right\| < \left\| \boldsymbol{x} - \boldsymbol{x_j} \right\| \quad \forall j \neq k \right\} \tag{2.1}$$

The grains are defined over a spatial region which includes the finely-meshed region of the workpiece as a proper subset to ensure that every element lies within a grain.

In the second step, the grains are assigned plastic properties. The simplest approach is to use a binary population of ‘phases’, i.e. each grain is treated as either ‘hard’ or ‘soft’. The present work uses five phases,[4] each with different flow properties, to better represent real metals. The proportions of the phases are roughly equal. Assigning a phase to each grain is then similar to the well-known problem of coloring the vertices of a graph using a set of specified colors [23]. However, there is an additional constraint arising from the fact that the resulting set of grains must possess a desired mean flow stress (or hardness H_0), i.e., one seeks a coloring $\{P\}$ that satisfies

$$\frac{\sum_{k=1}^{N} H(P(k)) * A(k)}{\sum_{k=1}^{N} A(k)} = H_0 \tag{2.2}$$

where N is the total number of grains, $P(k)$ and $A(k)$ are respectively the phase and area of the kth grain, and $H(m)$ is the hardness of the mth phase. The objective of the coloring algorithm is to ensure that grains having identical properties are separated from each other to the extent possible while satisfying this constraint.

In the third step, elements in the fine-meshed region are assigned to grains. Since each element lies in exactly one grain, it is convenient to work with element centroids; an element is considered to belong to a particular grain if its centroid lies inside the convex polygon defining that grain. The latter is a classical inside-outside classification problem in computational geometry [24], and easily implemented. Numerous other strategies for grain generation, partitioning and assignment of phases, including alternatives to the Voronoi process, are surveyed in Benedetti and Barbe [22].

2.2. Simulation setup

Sliding simulations are performed using the ABAQUS explicit dynamics solver [25]. An explicit solver is preferred because it handles contact well. The indenter/tool is kept fixed in the sliding (x) direction, while the workpiece/specimen is slid against it at a specified velocity V_0 of 5 mm/s. This velocity boundary condition is applied to nodes on the leftmost edge of the workpiece. Roller ($u_y = 0$) boundary conditions are applied to the lowermost nodes of the workpiece (Fig. 2a). Thermoplastic effects are negligible at these low velocities, allowing us to perform a purely mechanical analysis.

The rake angle α is a critical parameter for sliding. For the simulations reported here, five different values of α, $-80^\circ, -75^\circ, -70^\circ, -65^\circ$ and -60°, corresponding to $\theta = 10^\circ$, $15^\circ, 20^\circ, 25^\circ$ and 30°, are chosen (see Fig. 2a). These angles are representative of sliding contacts, asperities and die-workpiece

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[2] Some authors use the term ‘oligocrystal’ to describe such aggregates.

[3] Henceforth, the terms grain and pseudograin are used interchangeably while referring to simulations.

[4] The term ‘phase’ is used here to denote a subset of the workpiece with identical plastic flow properties.