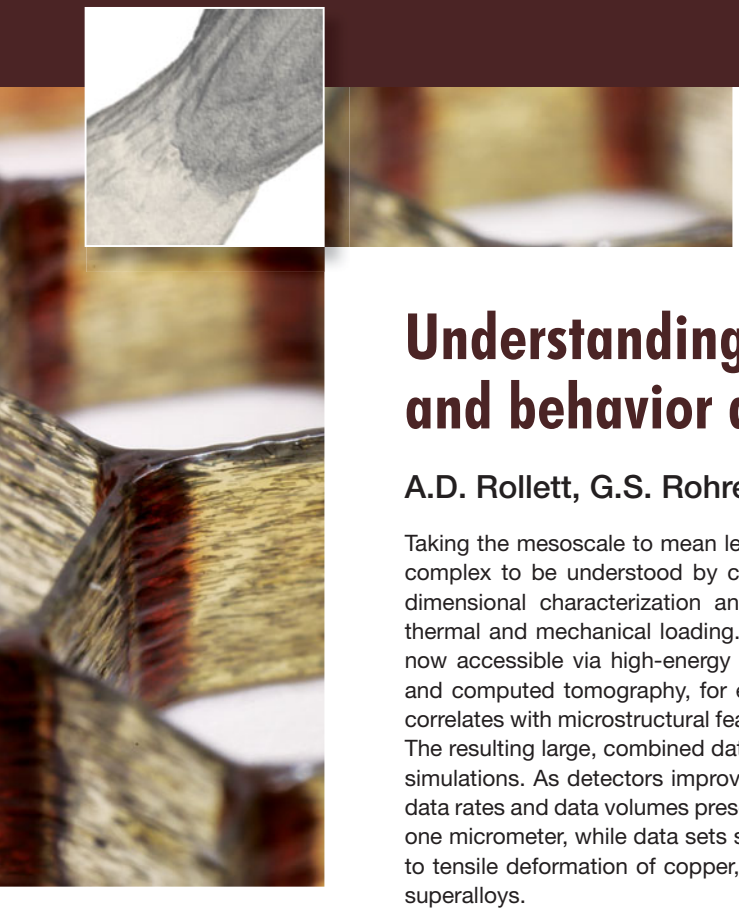

Understanding materials microstructure and behavior at the mesoscale

A.D. Rollett, G.S. Rohrer, and R.M. Suter

Taking the mesoscale to mean length and time scales at which a material's behavior is too complex to be understood by construction from the atomistic scale, we focus on three-dimensional characterization and modeling of mesoscale responses of polycrystals to thermal and mechanical loading. Both elastic and plastic internal structural responses are now accessible via high-energy x-ray probes. The combination of diffraction experiments and computed tomography, for example, is yielding new insights into how void formation correlates with microstructural features such as grain boundaries and higher-order junctions. The resulting large, combined data sets allow for validation of micromechanical and thermal simulations. As detectors improve in resolution, quantum efficiency, and speed of readout, data rates and data volumes present computational challenges. Spatial resolutions approach one micrometer, while data sets span a cubic millimeter. Examples are given of applications to tensile deformation of copper, grain growth in nickel and titanium, and fatigue cracks in superalloys.

Introduction

The mesoscale is a crucial realm in materials science, especially for polycrystalline materials. Put as succinctly as possible, a mesoscale property is an attribute of a material that cannot be straightforwardly constructed from properties at the atomic scale.[1] The prefix "meso-" implies being between the atomic and macroscopic scales, but the precise length or time scale where the break in understanding develops depends on the property. **Figure 1** illustrates the difference between traditional, reductionist approaches to science that attempt to deduce specific aspects of the underlying length or time scale from the larger scale behavior of systems, versus the constructionist approach, which is typical of mesoscale science, of seeking to build up properties by moving up the time and length scales. This article attempts to explain where a few mesoscale challenges exist for structural materials and their properties.

As pointed out in **Table I**, the properties of perfect crystal lattices can be calculated, although there are significant exceptions. Linear elastic deformation, even of composite materials, can be computed quantitatively with good accuracy, for example. Many of the useful materials properties for engineering depend, however, on the properties of lattice defects, such as interstitials, dislocations, and interfaces. Dislocations, in particular, are well understood as individual defects where an example of a well-established method is the calculation of the Peierls stress required to move them through a lattice.[2] Plastic deformation presents challenges because it generates large dislocation densities on multiple slip systems. Through the formation of various junctions,[3] the dislocations interact in complex ways that lead to heterogeneous densities and patterning that continue to be the subject of active research. Anisotropic interactions of defects within grain neighborhoods further complicate determination of emergent mesoscale properties. Given the importance of defect populations and their spatial heterogeneity, it is evident that multimodal, multiscale characterizations of materials are crucial to improving our understanding. Equally important is the use of models to quantify understanding, but these models must be tested against detailed experimental data. Accordingly, this article attempts to explain where a few mesoscale challenges exist for structural materials and their properties.

Mesoscale characterization and modeling of deformation

Plastic deformation of metals and alloys has been studied for decades. From the perspective of materials science, plastic deformation is dominated at low temperatures by dislocation

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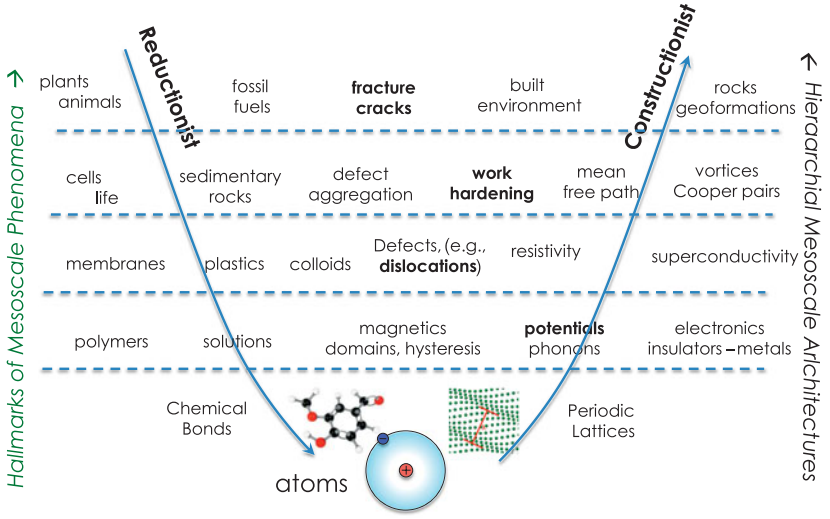

Figure 1. Diagram contrasting the more typical reductionist approach in science with the mesoscale science that results when the behavior at larger time and length scales cannot be constructed starting from the atomistic scale. This diagram has been adapted to illustrate the point that many aspects of the mechanical behavior of polycrystalline materials are strongly microstructure-dependent, and in many cases, cannot be computed from the properties of the underlying defects such as dislocations and point defects. Note: Bold text signifies properties, features, or defects that are relevant to this article. Courtesy G. Crabtree.

glide, which is crystallographic in nature (mechanical twinning is omitted here for lack of space). We refer in the usual way to single-crystal plasticity (CP) as the basis or model for understanding plastic (irreversible) deformation in polycrystals. Many aspects of deformation are well explained by CP. For example, deformation leads to preferred orientations of the crystals, known as texture, which is a direct result of the crystallographic nature of dislocation glide (e.g., $\{111\}\langle 110\rangle$ in fcc or $\{110\}\langle 111\rangle$ in bcc). Such textures result in anisotropic properties in polycrystals that reflect the convolution of single crystal anisotropy and the three-dimensional (3D) geometry of the texture; this is well established for a wide range of properties.[4] Why then is plastic deformation a significant mesoscale problem?

One motivation for studying metal deformation is the desire to quantitatively predict mechanical properties for applications in metal forming. As indicated above, quantification with CP works well and has been incorporated in finite element (FE) software as one example.[5,6] Another motivation, however, is to understand damage evolution. Damage covers a wide range of issues such as the accumulation of dislocation density—and increasing complexity of the dislocation networks during straining—and the development of orientation gradients,[7] voids,[8] and cracks.[9] Thus, another motivation for studying plastic deformation is to understand the rate of damage accumulation, its heterogeneities, and its relationship to microstructure. These phenomena illustrate the full complexity of the mesoscale: the single-crystal elements are understood, but the emergent behavior that dominates important properties are not well characterized or modeled.

Dislocation accumulation is equivalent to work or strain hardening, which is a far-reaching topic even at the single-crystal scale.[10,11] Although dislocation dynamics (DD) simulations exhibit strain hardening through tangling of dislocation networks,[10] understanding strain hardening in general requires a quantitative model for dynamic recovery—the loss of dislocation content as a function of strain, temperature, and strain rate—which is not yet available. That hardening remains a mesoscale problem might be regarded as simply a limitation of computing the evolution of dislocation networks in polycrystals over long periods (relative to the mean time between dislocation intersections); nevertheless, it serves as an example in which the sought behavior is sensitive to the details of interactions in large populations. Dislocation accumulation is almost always heterogeneous and has been much studied in terms of cell structure, both size[12] and morphology.[13] DD simulations show dislocation cell formation, provided that cross-slip is allowed to occur[11,14] (cross-slip means that a dislocation segment moves from its previous slip-plane onto a different one that is also compatible with [orthogonal to] the Burgers vector). Orientation gradients that develop with deformation can be regarded as higher-order heterogeneity due to dislocation accumulation, in which the polar nature

Table I. Mechanical properties and their accessibility.

Material Property	Computational Methods	References, Comments
Elastic moduli; point defect properties; Peierls stress for dislocations	Density functional theory	Generally accepted as reliable for a wide range of materials
Yield strength with anisotropy, temperature, and strain rate dependence	Dislocation dynamics (DD); crystal plasticity	Generally accepted as feasible for certain materials and composition ranges
Damage nucleation in plastic deformation; strain hardening; ductility	Molecular dynamics (MD) for void nucleation; DD for strain hardening and dislocation patterning	MD is limited to short physical times; DD limited to isotropic, symmetrically oriented single crystals. For damage, fully quantitative models lacking.
Stress corrosion cracking (SCC); fatigue crack initiation	DD has been applied to slip accumulation as a preliminary stage of crack formation. Mesoscopic models required for SCC.	No obvious path from first-principles calculations to prediction of this class of property.

of dislocations is apparent and concentrations of dislocations appear with a net rotation across dislocation wall structures.

In situ experimental measurements of dislocations and dislocation evolution in bulk polycrystals is extremely challenging. Transmission electron microscopy, combined with tomographic reconstruction, can image dislocations in 3D,[15] but controlling boundary conditions for mechanical deformation is challenging. Differential-aperture x-ray microscopy (DAXM) is able to map orientations in detail, but not at the level of individual dislocations.[16,17] Recent work using coherent Bragg diffraction imaging has succeeded in tracking individual dislocations in nanoparticles,[18] and this work may point the way toward similar, even more ambitious measurements in polycrystalline systems. Such measurements of elastic distortion fields around dislocations and collections thereof would provide vital evidence that could be used to inform DD and other types of simulations.

Even with the above limitations, it would be desirable to simulate polycrystal deformation with DD. However, apart from system memory limitations for practicable simulations, rules and models are lacking for the interaction of dislocations with interfaces. Examples of dislocation–interface interactions using atomistic level molecular dynamics are available,[19] but these simulations are limited in size and, especially, in strain.[20,21] Thus, while it is possible to understand hardening behavior qualitatively in the constructionist sense, quantitative derivation of polycrystal behavior from this starting point is not yet possible.

At the scale of polycrystals, orientation gradients are readily measured via orientation mapping, more easily on a surface with electron backscatter diffraction (EBSD),[22] but, with more effort, also in the bulk using near-field high-energy diffraction microscopy (nf-HEDM),[23] 3D x-ray diffraction,[24] or DAXM.[16] Examples of these measurements are discussed below.

Abstraction of dislocation motion in the form of CP embedded in the FE or fast Fourier transformation method removes the limitation of scale and permits a large enough part of the sample to be simulated to be able to match the boundary conditions. This allows comparison of orientation fields between experiment and simulation. A recent paper by Choi et al. described modeling of a microtensile test in an oligocrystal of nickel.[25] Reasonable agreement between the measured strain field (certain components of the tensor) and the calculated one was found, but it was not perfect. Beaudoin et al. looked in detail at the transition from elastic to plastic deformation in an aluminum (Al) alloy with nearly lamellar grains and found good agreement for both lattice strains and the transition into plastic flow.[26] Lim et al.[27] measured orientation change and strain in an oligocrystal of tantalum (Ta), compared the fields with CP-FE calculations, and found generally good agreement; interestingly, Ta is a material that does not readily form a dislocation cell structure. It is important to note that determining the relationship of damage accumulation with microstructural features (e.g., grain boundaries, triple lines, etc.) requires that the fields be accurately modeled. In this same paper,[27] the nominal boundary conditions (degrees of freedom for displacement at the ends of the gauge length) were varied: the calculated strain fields varied, but to a lesser degree than the difference with the measured fields. The orientation field was also measured and simulated for the same experiment; again, general agreement was found, as in the concentration of gradients adjacent to grain boundaries, but point-by-point agreement was not achieved.

Experiments that measure internal orientation fields in copper samples during tensile deformation have been performed with nf-HEDM at the Advanced Photon Source at Argonne National Laboratory.[23,28] **Figure 2** summarizes results showing a selected layer of the orientation field at different strain levels and computed tomography (CT), which reveals successive necking of the sample's gauge region, as well as internal void development at high strains. The increase in orientation spread in two particular grains (numbered 2 and 15) shows distinct behavior with one broadening, while the other splits into two separate orientation clusters. The orientation broadening is reflective of the general increase in orientation variations in grains throughout the polycrystal, as illustrated in Figure 2d. This combination of nf-HEDM and CT represents an example of multimodal measurement made possible by nondestructive high-energy x-ray methods. Other examples are beginning to appear in the literature.[29]

From the data set of Figure 2, a single layer was selected in the center of the gauge length for comparison at different strain levels, and with CP simulations, which were performed with a spectral method well suited to using orientation maps measured on a regular grid as input.[30] As with other comparisons, the orientation change was well captured by the simulations at the statistical level. However, the lattice rotations of individual grains (in the frame of the sample) were smaller in magnitude in the experiment as compared to those for the simulation, and the data scatter was substantially larger. When the orientation gradients were compared between experiment and simulation, substantial differences were found. This latter difference was later found to be due to the limited spatial resolution of the nf-HEDM technique which is about 2 μm. When more detailed EBSD measurements with 0.2-μm spatial resolution were made on cross sections through the tensile sample, better agreement with the simulations was found, and the orientation gradients were found to concentrate next to grain boundaries, as observed in the simulations.[7] Recent advances in dark-field microscopy using synchrotron x-rays have demonstrated that mapping orientation gradients at the subgrain (i.e., submicron) scale is becoming feasible.[31,32]

To summarize, plastic deformation and the reorientation of the crystal lattice at the scale of gradients within individual grains remains a mesoscale challenge, because the currently available evidence is that continuum scale simulations in general cannot capture the spatial distribution of strain and orientation adequately, and simulation tools that are more directly based on the behavior of the underlying defects

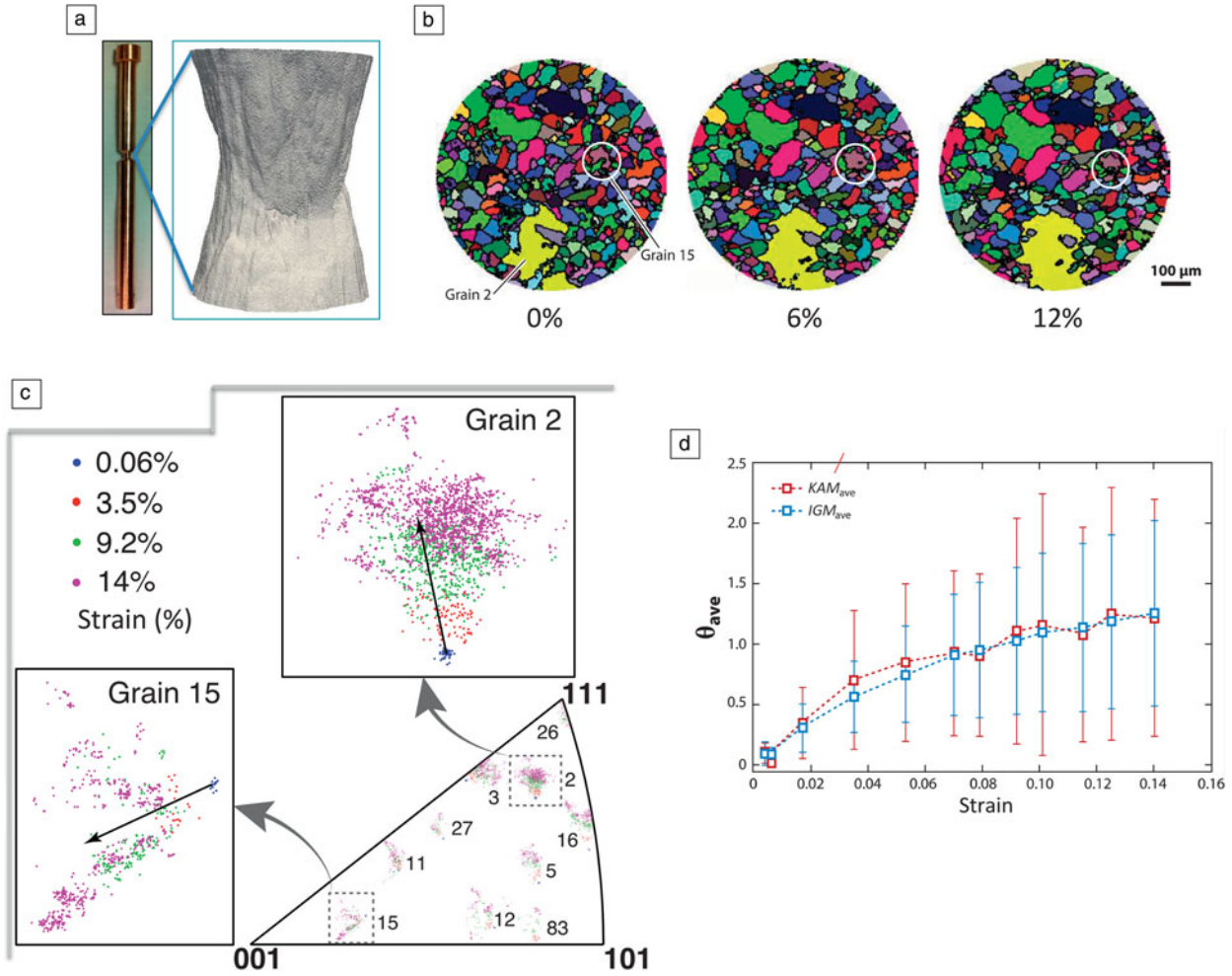

Figure 2. (a) An image of the (left) copper tensile sample and (right) a tomographic image of the waisted gauge section that was tracked with near-field high-energy diffraction microscopy (nf-HEDM) and computed tomography as the specimen necked. The initial diameter of the gauge section was 1 mm. (b) Voxel-based lattice orientation maps from nf-HEDM of a selected cross section show how individual grains are tracked between successive strain steps (0%, 6%, and 12%); grains 2 and 15 are marked. (c) Voxels in a set of 10 large grains tracked in an inverse pole figure; the exploded views emphasize how initial orientations (blue) expand into clouds of orientations as strain increases (red, green, purple). The thin black arrows indicate the change in the average orientation of each grain. Grain 2 spreads rather uniformly, whereas grain 15 appears to bifurcate into two orientation regions. (d) Orientation variations within grains averaged over the 150 largest tracked grains: KAM_{ave} is the globally averaged grain average of the local kernel average misorientation; IGM_{ave} is the average of the misorientation of each point from the average orientation of the associated grain.[7,23] Vertical bars are standard deviations across 150 grains. Note: θ_{ave}, average value at each strain step of either the *KAM* or *IGM*.

(i.e., dislocations) are unable to address polycrystal deformation problems.

Turning our attention to another aspect of damage accumulation, under many conditions of plastic deformation, voids form inside a material well before the macroscopic ductility limit (i.e., fracture). In most engineering materials, the microstructural location for void initiation is coarse second-phase particles, which may either crack or decohere from the matrix.[33] In standard tensile tests measuring strength and ductility, the first voids form in the center of the neck where the triaxiality* is highest. Similarly, in two-phase steels with particles or regions of martensite that are harder than the surrounding ferrite, void formation typically starts at locations between hard particles, where the maximum principal stress is highest.[34] In single-phase metals, voids still form and under dynamic loading conditions, they form in large numbers wherever there is a large difference in plastic response across a boundary. Thus, in experiments to test spall strength, it is found that voids form most commonly on grain boundaries and that they tend to avoid low energy boundaries such as twin boundaries,[8] based on polished cross sections and EBSD characterization. Work is in progress to perform more detailed 3D experiments and simulations to verify and quantify these relationships.

* Triaxiality is defined as the quotient of the mean stress over the von Mises equivalent stress, where the latter is a standard measure of the deviatoric stress.

Thermal responses of microstructure in three and four dimensions at the mesoscale

Accurate prediction of mechanical properties requires a detailed knowledge of the polycrystalline microstructure in three dimensions as well as its evolution in strain or time, which represents the fourth dimension. At first glance, polycrystalline structures are straightforward. They arise from a coarsening process (i.e., grain growth), which is a natural consequence of grains that are smaller than the average tending to shrink relative to large ones. Because their surfaces have smaller inward-pointing curvatures, larger-than-average grains grow. Some characterization studies in 3D have been published in recent years, thanks to the availability of automated serial sectioning[35] and high-energy x-ray diffraction methods.[17,37,42,62] The main features of grain growth discussed here make it clear that this is another mesoscale problem.

1. The interfaces that possess excess free energy, and provide the driving force for grain growth, are anisotropic in energy and mobility. Although this was always clear from atomistic models of structure and properties, it was not until mesoscopic methods were used to collect the population statistics on large numbers of grain boundaries[38] that the dependence of the grain boundary energy on crystallographic type was found to follow a systematic trend in which, with one important exception, the excess energy is approximately the average of the energies of the two surfaces joined at each grain boundary, minus a binding energy. Notwithstanding this clear trend, no straightforward theory describes how energy varies with crystallographic type.

2. In most fcc metals, the energy of the coherent twin boundary, which involves a 60° ⟨111⟩ misorientation relation with a {111}-oriented interface, is more than an order of magnitude smaller than that of nearly all other grain boundary types. Consequently, these boundaries typically appear in the material as flat, planar interfaces. Twin boundaries often comprise one-third or more of the total grain boundary area. In the coincident site lattice framework, this misorientation relation is referred to as Σ3, although this designation does not include the {111} boundary normal designation (one speaks of "incoherent twin boundaries" as those with Σ3 misorientation, but not having a {111} normal). Twins arise mainly from recrystallization after plastic deformation,[39] and their presence enhances the fractions of related twin types such as Σ9 and Σ27. Although the phenomenology is clear, we lack a detailed model of twin formation that accounts for all of the facts.

3. Comparisons of grain boundary populations with theoretical calculations of energy[40] show strongly negative correlations for boundary types with lower-than-average energy (i.e., more boundaries with lower energies). This is an expected result because, in most polycrystals, grain boundaries meet in sets of three along triple lines, where a force balance exists in local equilibrium. This force balance determines the dihedral angles between the boundaries, which, in turn, determines the local curvatures and thus, the relative rates at which boundaries move. Simulations have demonstrated that this force balance leads to more rapid elimination of high energy boundaries compared to lower energy boundaries.[41] Nevertheless, the anticorrelation only holds for the lowest energy boundaries with large populations, and wide scatter exists at the upper end of grain boundary energies.

This summary suggests that grain boundaries are well understood. However, some gaps in our understanding and challenges remain, as already mentioned. There is no direct comparison that has been performed between experimentally determined evolution of the grain structure in 3D and computational prediction based on fully validated anisotropy of energy and mobility, which would represent validation of grain growth models.

There are a few data sets with multiple 3D orientation maps obtained during grain growth at successive times for metallic nickel[42] and ceramic $BaTiO_3$.[43] For nickel, it is observed that annealing twins form at specific triple junctions where the insertion of the twin reduces grain boundary energy despite increasing total boundary area.[62] For the titanate, abnormal grain growth is observed in a narrow temperature interval. However, only one study has been published to date that makes a direct comparison to a 3D grain growth model;[44] good agreement is obtained in some areas, although one conclusion is that further research is required to incorporate better descriptions of grain boundary anisotropy. The small amount of work on 2D systems suggests that anisotropy[45] must be incorporated in order to obtain reasonable agreement. Simulating grain growth, however, requires knowledge of both energy and mobility. Recent theoretical work on grain boundary mobilities[46] shows that although a large subset of boundary types exhibit thermally activated behavior, there is also a large fraction of boundary types that exhibit essentially no thermally activated motion and some types that undergo roughening transitions.[47]

Clearly, much research is required in this area. Grain growth represents a mesoscale problem that involves translating our limited understanding of the properties of boundaries at the atomistic level into quantitative predictions of boundary dynamics and consequent microstructural evolution. In addition to the purely interface-driven coarsening (i.e., grain growth) described here, at least as important are boundary motions being driven by the reduction of stored-energy-driven recrystallization.[63]

Mesoscale characterization and modeling of fatigue cracks

Fatigue, as a particular mode of inducing plastic deformation, has also been the subject of intense study for several decades, and substantial success has been obtained in the quantification of fatigue crack growth.[48,49] As noted in Table I, cracking under most circumstances is characteristic of mesoscale problems because of the challenge of building quantitative models from basic material properties. The ultimate challenge is to develop quantitative models of component lifetime under realistic fatigue loading conditions. In many cases, a significant fraction of the lifetime is associated with fatigue crack initiation.[50] The word "initiation" is used because, from

an engineering perspective, the practical definition of initiation involves the identification of a crack through some sort of nondestructive examination and an arbitrary threshold for separating slip steps from cracks. Once a detectable crack exists, standard techniques can be used to predict its growth based on knowledge of the loading conditions. From a scientific perspective, this situation is unsatisfactory, because we have only an approximate understanding of how cracks start and how to predict their growth when they are short compared to the scale of the microstructure. The propagation path is often highly irregular. Hence, we divide the problem into two stages, the first of which is the initiation of the crack and second is the propagation of microstructurally short cracks.

In terms of physical metallurgy, crack generation under cyclic loading has been well studied in single-phase metals such as copper. Dislocations move back and forth on their slip-planes, but interaction between them and cross-slip from one slip-plane to another leads to the formation of characteristic microstructures that are often described as ladder-like. Once the cyclic stress–strain behavior has attained saturation in the characteristic hysteresis loop, irreversible motion sets in.[51] The exhaustion of hardening allows continued cycling to concentrate the slip in specific locations; given enough accumulation of slip steps, a crack forms. To this point, the problem is partially accessible from first principles in the sense that the motion of the relevant defect, the dislocation, can be simulated with DD.

Déprés et al.[52] have shown how the formation of a stationary stress–strain loop can be simulated for a single-slip system: such saturation in the cyclic stress–strain behavior is a precondition for crack formation. Earlier work with a 3D model showed how slip steps arise from the development of multipolar dislocation walls in a persistent slip-band structure,[53] and this has been extended to modeling the early stages of fatigue crack growth.[54] Further experimental evidence for the importance of microstructure, orientation, and dislocation interactions with interfaces can be found in the work by Dehm's group on thermal cycling of thin films on substrates in which differential thermal expansion induces significant stress and plastic strain in each cycle. For aluminum films grown with a strong texture with ⟨111⟩ parallel to the film normal, the surface remains smooth after thousands of cycles; in polycrystalline films with a weak texture, surface ridging develops rapidly, and the texture changes.[55]

Unfortunately, such an approach bears little resemblance to engineering alloys that almost always contain significant densities of particles. It is clear that different classes of materials exhibit different behaviors. Fatigue crack initiation in aluminum alloys, for example, is dominated by cracking of brittle, so-called constituent particles,[56] which are found in sizes of well over 1 μm. The coarser the particle, the more likely it is to crack within a few cycles. The more difficult quantification is when the crack grows into the surrounding matrix. Crack initiation in nickel-based superalloys has been shown, at the statistical level, to be dominated by slip accumulation next to annealing twin boundaries.[57] The twin boundaries are important because they are barriers to slip on all systems except those that run parallel to the twin plane, which helps to explain why the length of the twin boundary on the surface, directly related to grain size, is related to the probability of initiation.[9]

For crack initiation, DD has been of some help because the motion of large numbers of dislocation segments can be simulated. Simulations of slip-step formation[58] show that materials with shearable particles, characteristic of the smaller hardening particles in nickel alloys, generate slip steps after fewer cycles than in materials with larger, nonshearable particles. The DD simulations are confined to single-crystal simulations, however, which means that we are as yet unable to bridge the gap between this scale and the effects of polycrystal microstructure, such as that of grain boundaries.

Once a crack has formed, its growth is typically highly irregular until it becomes large enough compared to the microstructure that it grows perpendicular to the axis of the maximum principal stress. Gangloff and co-workers[59] have demonstrated that at least in Al alloys, the crack path rarely follows a precise crystallographic trajectory such as slip-planes or a preferred cleavage plane. They point out that, despite expectations from CP, environmental factors such as moisture measurably affect aluminum alloy crack growth rates and morphologies and that this is likely to be the case in other alloys.

There have been a small number of recent examples of full 3D characterization of such microstructurally short cracks. Buffière's group used CT combined with diffraction contrast tomography[37] to measure both the morphology and crystallographic orientation of the crack-adjacent grains in a titanium sample.[48] Suter's group has made measurements using nf-HEDM[36] and tomography spanning a region of ~500 μm around the initiation point of a fatigue crack in a sample of nickel-based superalloy Rene88DT.[60] Efforts to model the path of the crack are ongoing. **Figure 3** shows a 3D volume surrounding a grain-sized crack in a nickel-based superalloy that was measured with nf-HEDM.[9] This volume was used to instantiate CP-FE calculations that verified that a hot spot in accumulated dislocation slip is found in the simulation at the same location as a known microcrack.[61] From the same sample, multiple microcracks were characterized, all parallel to annealing twin boundaries, from which it was deduced that both twin orientation (in relation to the applied stress) and twin length are factors in crack initiation.[9] Also using nf-HEDM, Spear et al. measured several hundred micrometers of a crack in an aluminum alloy.[49] Detailed modeling of the propagation path and similar efforts are being developed.

These examples of short-crack propagation characterization all required the use of recently developed high-energy x-ray probes implemented at third-generation light sources which illustrates the utility of these advanced tools for validating computational models. Despite the lack of simulations that attempt to model the details of crack advancement, we have reviewed them here because they demonstrate how making progress on this important issue requires further

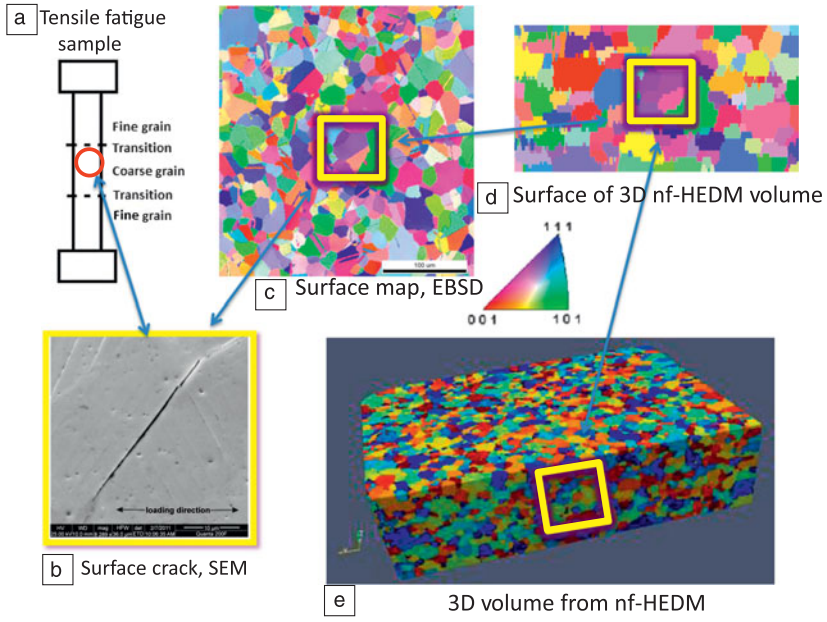

Figure 3. Illustration of the value of multimodal imaging. (a) The thin-sheet sample of the nickel-based superalloy was subjected to tensile fatigue. (b) Replicas supplemented by scanning electron microscope (SEM) identified surface cracks. (c) Orientation scanning (electron backscatter diffraction [EBSD]) in the SEM mapped out the area around the surface crack in detail after the sample had been measured with a near-field high-energy diffraction microscope (nf-HEDM) in (d) three dimensions (around the same crack), approximately 600 μm × 800 μm × 240 μm. False colors are mapped from the Rodrigues vector components specifying the orientation at each point. (e) The three-dimensional (3D) measurement permits the micromechanical fields around the crack to be calculated.[9]

advances in experimental, theoretical, and computational tools. To run an FE simulation with CP over many strain steps requires computation times on the order of a few days when the microstructure contains dozens or hundreds of grains and is geometrically complex enough to require verified, reliable meshes with many millions of degrees of freedom. Thus, new measurement tools are motivating the development of new computational tools.

Summary

Substantial progress in mesoscale experiments and related modeling has been demonstrated, while at the same time, much remains to be investigated and learned. Plastic deformation results in heterogeneous lattice rotation inside grains, which is not accurately simulated with current tools. Strain hardening similarly presents a challenge for quantitative modeling because it involves the behavior of large populations of dislocations. Grain growth depends on interface motion, which is difficult due to the lack of validated understanding of properties such as grain boundary energy and mobility. Fatigue cracking (and most cracking problems) depends on the heterogeneity of slip and on the asymmetric accumulation of surface displacement, another challenging mesoscale problem. In each of these cases, mesoscale science will continue to benefit from and motivate new types of measurement capabilities; with these new capabilities, associated computational tools are being developed to extract responses from combined multimodal data sets. Further developments will bring new methods for comparing, on local and statistical levels, *ex post facto*, and in real time, the experimental observations and large-scale computational models.

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