

# Alloy design for mechanical properties: Conquering the length scales

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Predicting the structural response of advanced multiphase alloys and understanding the underlying microscopic mechanisms that are responsible for it are two critically important roles that modeling plays in alloy development. The demonstration of superior properties of an alloy, such as high strength, creep resistance, high ductility, and fracture toughness, is not sufficient to secure its use in widespread applications. Still, a good model is needed to take measurable alloy properties, such as microstructure and chemical composition, and forecast how the alloy will perform in specified mechanical deformation conditions, including temperature, time, and rate. Here, we highlight recent achievements using multiscale modeling in elucidating the coupled effects of alloying, microstructure, and mechanism dynamics on the mechanical properties of polycrystalline alloys. Much of the understanding gained by these efforts relies on the integration of computational tools that vary over many length scales and time scales, from first-principles density functional theory, atomistic simulation methods, dislocation and defect theory, micromechanics, phase-field modeling, single crystal plasticity, and polycrystalline plasticity.

## Introduction

For at least a century, modeling has played an integral and critical role in alloy design. Two-dimensional maps, equations, and rules are some of the most popular and utilized forms of modeling. Ashby maps have facilitated materials selection, enabling comparisons between classes of alloys against measurable performance indices, such as specific stiffness and yield strength.<sup>1</sup> The Hall–Petch scaling law has been used through the years to relate material strength/hardness to grain size in a polycrystal.<sup>2,3</sup> The Hume–Rothery rules are widely used to guide the choice of alloying elements to indicate whether the alloy will be single or multiphase.<sup>4</sup>

While the insights afforded by straightforward rules, expressions, and maps are greatly appreciated, there continues to be a need to develop better materials models. Alloy design has been stretched to encompass more than simply choosing which and how many solute atom(s) to add. Additions of just a few percent of alloying elements can profoundly affect the activation of nanoscale mechanisms (operating over Ångström to nanometer scales) when the alloy is deformed. With heat treatment and mechanical processing, these atomic-scale element

additions can affect the evolution of the internal microstructure (characteristic length scales > nanometer scale). The resulting alloy microstructures are often complex, consisting of multiple phases with each phase containing more than one type of precipitate, particle, or interface. Changes in any of these features can, in turn, influence a broad suite of critical bulk structural properties (samples > millimeter scale), such as strength, ductility, fatigue, fracture, and creep. In order to continue to benefit the design and optimization of alloys, materials models need to be multiscale, spanning from atoms to the continuum.

A full-spectrum, “atoms-to-continuum,” multiscale materials model (MMM) for alloy design, however, does not exist. Atomic-scale models that treat a polycrystal as a collective arrangement of atoms exist. Continuum models that treat the sample or structure as a deformable continuum also exist. The modeling components that are missing lie in the intermediate scales, between the nanometer and millimeter scales, collectively referred to as the mesoscale. Crossing the vast mesoscale gap is where MMM meets its greatest challenges.

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**Figure 1** displays a current view on mesoscale MMMing for advanced alloys. At its core (central circle), a mesoscale MMM intends to benefit alloy design by aiding in the understanding, processing, and design of new materials. These MMMing efforts tend to pursue one of three goals (intermediate ring). Some MMMs are built to improve and discover deformation mechanisms. Other MMMs are developed to simulate microstructural evolution under a specific manufacturing process so they can identify pathways to achieve target microstructures. Last are MMMs that focus on determining microstructure–materials response relationships in an effort to address the question, “which microstructures are the ‘right’ ones?” At the periphery (Figure 1) lie the multitude of mesoscale multiscale models to date that treat more than one length scale in the mesoscale spectrum. This article aims to highlight some of these MMMing achievements for alloy design.

### Coupling the thermodynamics and mechanics of precipitation

Precipitation hardening is well established as one of the most efficient strategies to increase the yield strength of alloys. Precipitates are metastable intermetallic particles with sizes ranging from a few to a few hundred nanometers that appear during aging of alloys. Improvements in alloy strength depend on the precipitate size, shape, and spatial distribution, as well as how moving dislocations interact with them. In their article in this issue, Nie and Wang<sup>5</sup> highlight many recent

achievements in precipitation design for improved lightweight alloys.

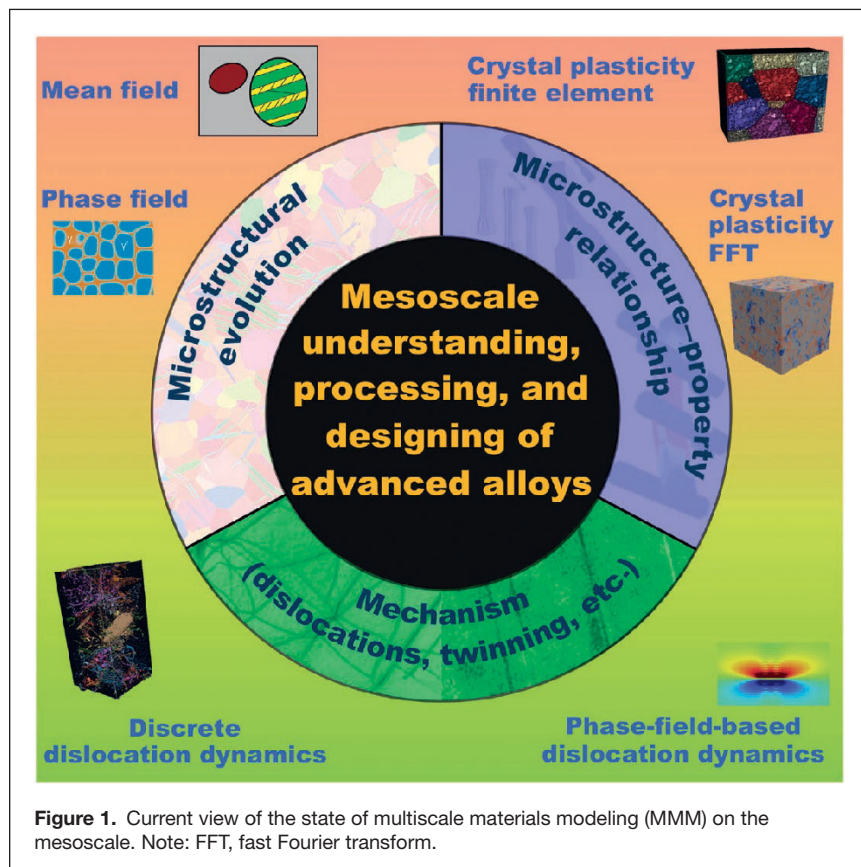
Multiscale modeling strategies can aid in the design of novel precipitation hardened alloys by replacing costly experimental trial and error approaches. Recently, one such MMM was built for the precipitation process in Al-Cu alloys.<sup>6–11</sup> At its foundation is an analysis of thermal stability for each kind of precipitate, which is accomplished by first-principles calculations of the Helmholtz free energy.<sup>7</sup> Precipitate nucleation and growth are then predicted, respectively, via classical nucleation theory and phase-field mesoscale simulations (**Figure 2**).<sup>7,8</sup> The former is used to predict the initial dimensions and shape of the precipitate nucleus. When nucleation is homogeneous, it calculates the chemical, interfacial, and elastic driving forces using computational thermodynamic data, first-principles calculations, and lattice correspondence during the transformation. In the likely situation of heterogeneous nucleation—that is, when the stress fields from other precipitates, dislocations, or defects, can alter the nucleation process—such stresses can be taken into account in the multiscale framework. Once the initial dimensions and shape of the precipitate nucleus have been determined, growth of the precipitate to its stable shape is calculated using the phase-field method.<sup>8</sup>

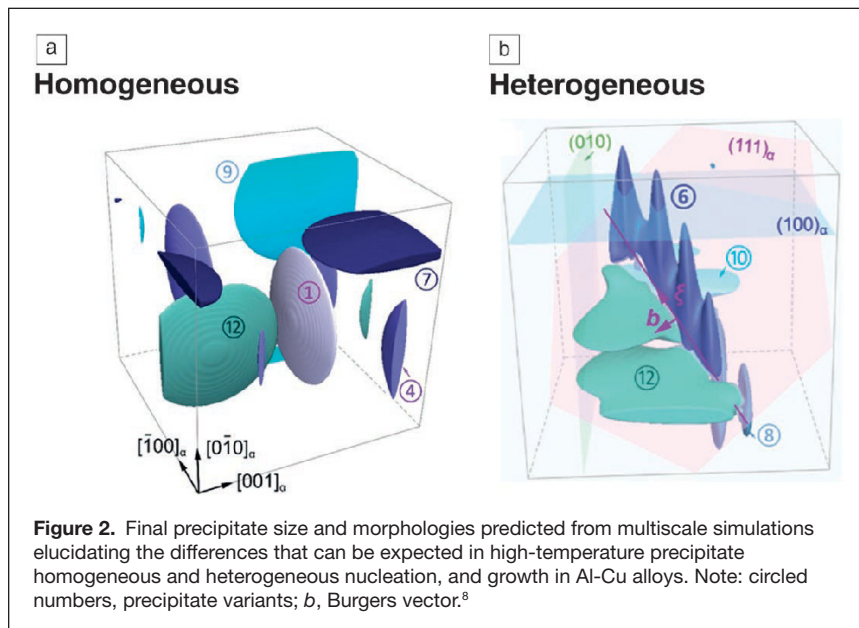
Multiscale simulations from this strategy can reveal the stability and growth sequences of precipitation, as well as the expected final precipitate microstructure. Figure 2 demonstrates the profound effect dislocations can have on the final equilibrium shape of precipitates, being flat disks when nucleation is homogeneous versus cones and platelets with morphologically rough edges when nucleation is heterogeneous.<sup>7,8</sup>

### Chemo-mechanical interactions between gliding dislocations and precipitates

The amount of strengthening provided by precipitates in an alloy depends on atomistic and mesoscale aspects of the mechanisms used by dislocations to bypass these precipitates. While a few bypass processes have been proposed and studied, the mechanism is usually not known *a priori* since it depends on strong couplings among the geometric, chemical, and mechanical properties (e.g., crystal structure, composition, stiffness, lattice orientation) of the precipitates.

Ni-Al-based superalloys provide one prominent example of the need to consider both mechanical and chemical aspects in the processes underlying dislocation/precipitate interactions. While alloying provides for a microstructure consisting of precipitates (e.g., the  $\gamma'$  phase), further improvements in strength could be





gained by adding solute elements, such as W, Re, Co, and Cr. However, solute segregation to defects, such as dislocations and stacking faults<sup>12–15</sup> could instead lead to precipitate dissolution, enhanced directional coarsening (“rafting”), and degradation of mechanical properties. Due to the chemo-mechanical couplings involved, calculation of the mechanisms and associated critical energies and stresses required by dislocations to bypass the precipitate call for a multiscale strategy.

In the last few decades, multiscale models combining atomistic calculations and phase-field modeling have been developed to simulate dislocation motion.<sup>16–18</sup> To treat alloys, the energetics used in the phase-field dislocation simulations have been advanced to include chemo-mechanical couplings.<sup>19,20</sup> In these models, the roles played by morphology and chemistry in the mechanisms that underlie dislocation–interface interactions are encompassed in the energetic terms used in the master energy function of the phase-field method.

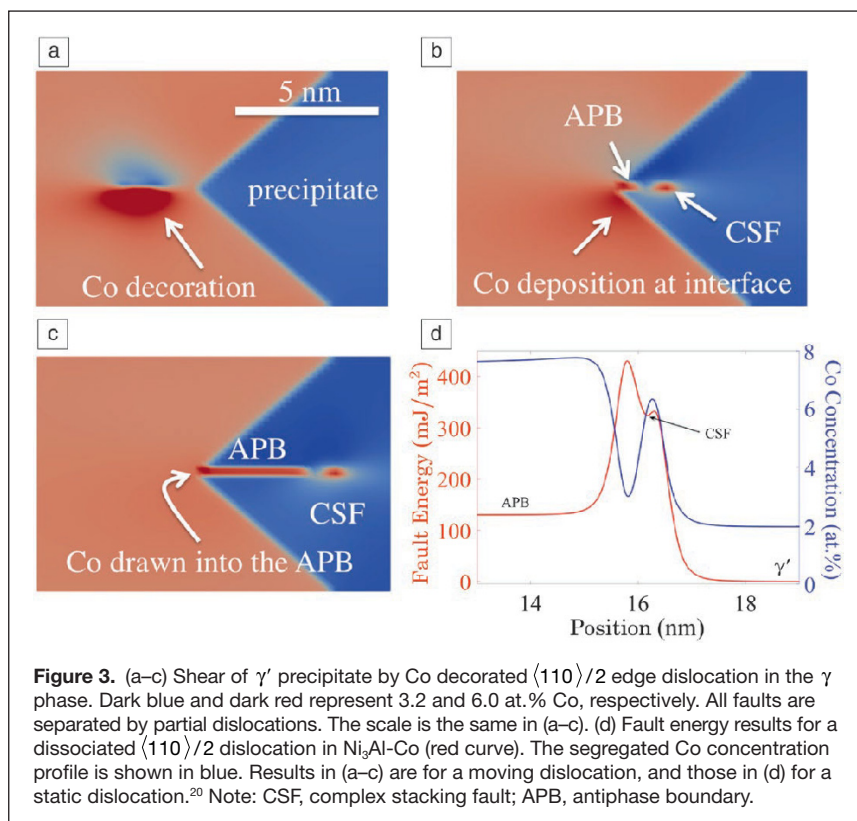
**Figure 3** shows a result from one recent example in this class.<sup>20</sup> The MMM combines a general phase-field-based chemo-mechanical methodology<sup>21</sup> with phase-field dislocation modeling to simulate dislocation shearing of a precipitate in Ni-Al-Co. Under an applied stress, the dislocation glides in the matrix toward the precipitate. Before reaching the precipitate, the dislocation dissociates into two Shockley partial dislocations and is decorated by Co (Figure 3a). At the  $\gamma$ – $\gamma'$  interface in Figure 3b, these partials recombine into a perfect edge dislocation before they enter and

shear the precipitate. As the dislocation glides into the  $\gamma'$  precipitate, it deposits Co on the  $\gamma$ – $\gamma'$  interface (Figure 3b) as well as drags Co into the precipitate (Figure 3c). Ultimately, as seen in Figure 3d, Co segregation enriches the faults left by the shearing process and depletes Co in the precipitate  $\gamma'$  matrix.

The coupling between dislocation shearing and solute segregation could promote precipitate dissolution, directional coarsening (“rafting”), loss of strength, and lifetime reduction. The insights obtained by such multiscale simulations can be useful for optimizing the alloying composition to delay or inhibit such effects.

### Moving dislocations across scales

One computational approach that can provide understanding and prediction of the deformation of alloys is the three-dimensional discrete dislocation dynamics (3D DDD) simulation method. This mesoscale technique was developed to model plastic deformation as a result of collective motion of many dislocations gliding in a crystal.<sup>22–25</sup> In recent years, DDD has been applied to model microstructure-response relationships in superalloys and, in particular, to explore the effects of several dislocation/precipitate interactions in a crystal.<sup>26</sup>



**Figure 4a** shows the predicted response of Ni-based superalloys as a function of the size of cuboidal precipitates within single crystals of the polycrystalline alloy. In these calculations, this mesoscale technique advantageously accounts for randomness in the distribution and shapes of the precipitates in the crystal, the evolution of a collection of dislocations, and the numerous precipitate–dislocation interactions. The model reveals that the precipitate size effect is due to a change in the dislocation–precipitate bypass mechanism with increasing precipitate size (see Figure 4b–c).

Three-dimensional DDD simulations have been successfully used to quantify many other important microstructure–strength relationships, such as a nearly independent relationship with grain size (compared to the strong precipitate size effect), a linear increase with precipitate volume fraction, and an approximately square-root relationship with antiphase boundary (APB) energy. Such strength–microstructure relationships can improve calculations of deformation and failure in simulations that treat larger length scales and time scales, such as crystal plasticity (CP) simulations. Three-dimensional DDD simulations have also been advanced to track the formation and destruction of intrinsic and complex faults,<sup>27</sup> processes that are strongly dependent on superalloy composition. Another noteworthy extension is the inclusion of misfit stresses resulting from significant lattice mismatch between two phases.<sup>28,29</sup>

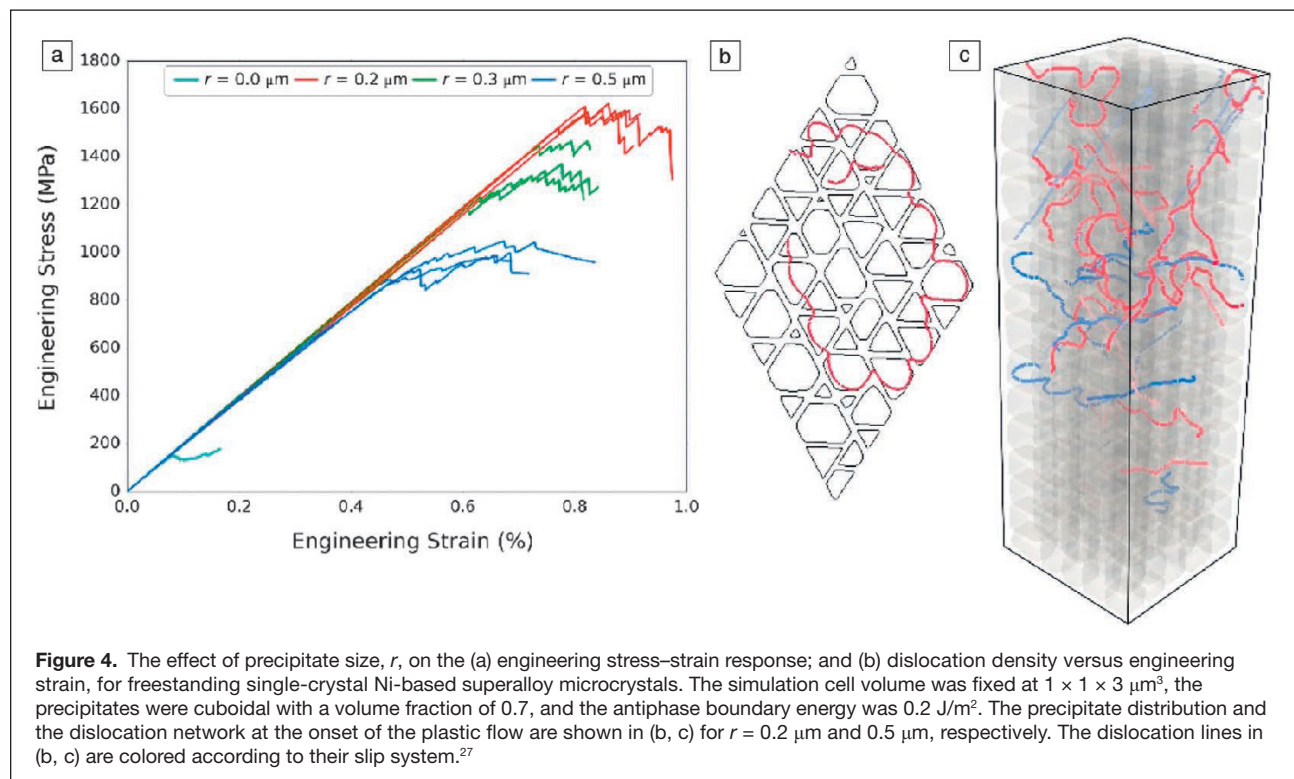
### Using alloying to improve formability in magnesium

Hexagonal close-packed (hcp) metals, such as Mg, Zr, and Ti and their alloys, are being considered for a broad range of

high-performance structural applications.<sup>30,31</sup> They bear many attractive intrinsic properties, such as low specific density, fatigue resistance, biocompatibility, corrosion resistance, and radiation resistance. Successful incorporation of hcp alloys into engineering designs has been hindered because their structural behavior is challenging to predict.

Mg alloys represent one prominent and current example. For several decades, they have drawn attention as an ideal candidate for lightweight transportation due to their low density and high specific strength.<sup>32,33</sup> However, their poor formability at room temperature limits widespread use.<sup>34</sup> For Mg, there are several modes of slip, with the common modes being basal  $\langle a \rangle$ , prismatic  $\langle a \rangle$ , and pyramidal  $\langle c + a \rangle$ . Each is distinct in terms of crystallographic slip plane and direction as well as critical resolved shear stress (CRSS) to activate it.<sup>35,36</sup> Poor formability is a consequence of the significant differences in slip mode CRSS.

Alloying can increase or diminish CRSS differences. In recent work, a multiscale polycrystal plasticity model (MPPM) was employed in an attempt to comprehensively explore solute effects on the CRSS values and on formability.<sup>37</sup> At the highest length scale, the model utilizes a micromechanics formulation to relate the deformation of an aggregate of crystals to the deformation of an individual crystal. A grain-scale model for deformation twinning has been used to account for division of a crystal into twinned and untwinned crystalline domains. Each domain is permitted to deform by crystallographic slip. Finally, the CRSS values for slip for a particular alloy are used as input and these are allowed to evolve with local amounts of slip strain.



CRSS differences among slip modes can be quantified via a plastic anisotropy (PA) measure. Presuming that basal slip is the easiest slip mode, typically the case for Mg alloys, this measure is given as:

$$PA = \frac{\tau_0^{\text{Prismatic}} - \tau_0^{\text{Basal}}}{\tau_0^{\text{Twin}} - \tau_0^{\text{Basal}}}, \quad (1)$$

where  $\tau_0$  is CRSS and the superscript indicates the slip or twin mode. MPPM was employed to simulate the plastic response and extract quantitative measures associated with formability for a number of high-performance Mg alloys ranging broadly in PA measure.

**Figure 5a** presents the calculated ratios of the tensile yield stress to the compressive yield stress. Overall, the values are consistent with experimental measurements.<sup>38–44</sup> The important finding in **Figure 5a** is the strong relationship between the calculated tension-compression yield stress ratio and the plastic anisotropy PA measure.

As another measure of formability, the MPPM was used to calculate the polycrystal yield surfaces (PCYSs) of many alloys. A yield surface is a five-dimensional surface in the six-dimensional space of stresses. When the stress state lies on the surface, the material is said to have reached its yield point and to have become plastic. **Figure 5b–c**<sup>37</sup> presents calculated  $\pi$ -plane projections of the PCYSs for pure Mg and two different Mg alloys. A remarkable feature is the broad range of yield stresses that can be achieved via alloying. The Mg4Li alloy (96 wt% Mg and 4 wt% Li) has the smallest PCYS (**Figure 5b**) and the ZW41 alloy (0.4 wt% Zr, 3.7–4.3 wt% Y, 2.4–4.4 wt% Nd, with the rest being Mg) has one of the largest (**Figure 5c**). Asymmetries in the PCYSs reflect that plastic anisotropy, and as anticipated, the level of asymmetry, scales with the

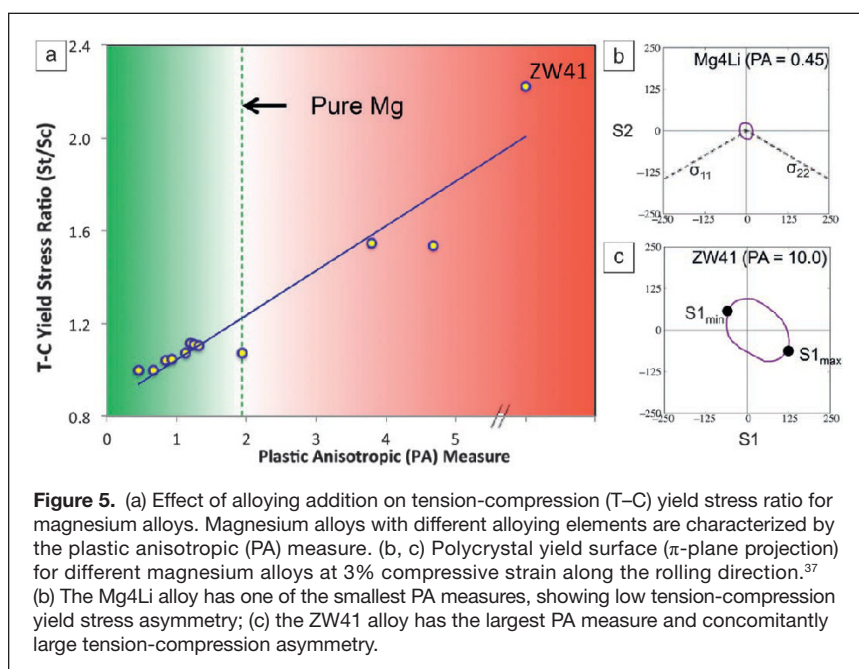
PA measure. In revealing a strong correlation between the PA measure for slip and key measures for formability, MPPM introduced a new measure that can be used to screen for alloys that would potentially be formable.

### Hierarchical microstructure-sensitive structural properties

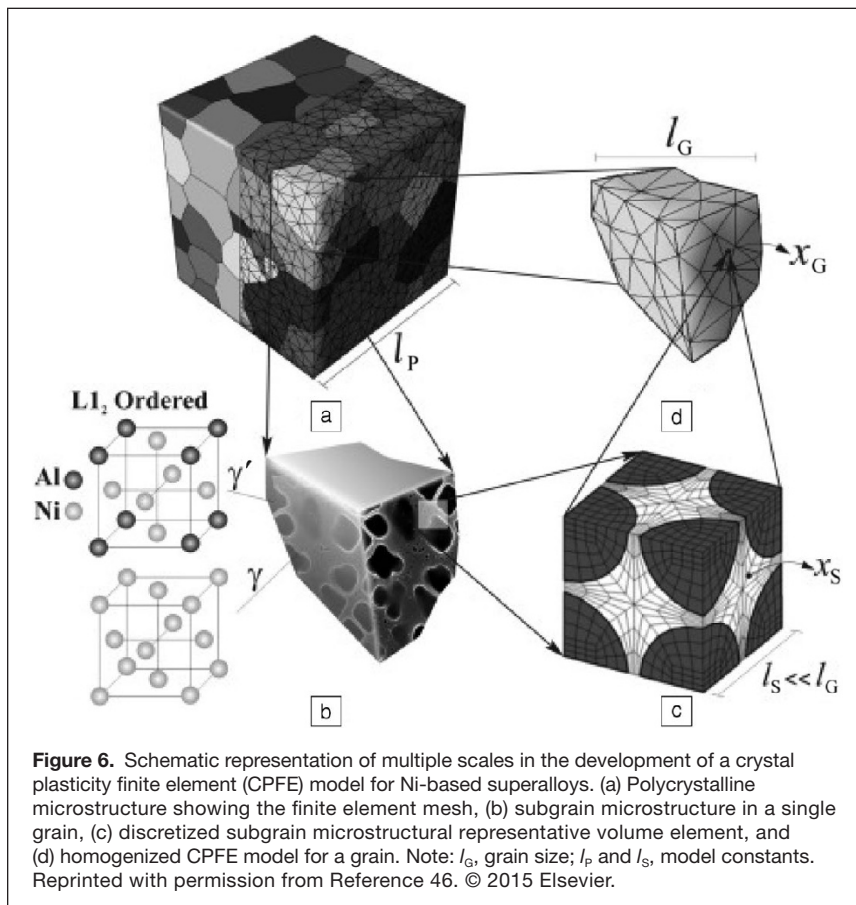
The structural properties of today's most advanced alloys are highly dependent on a hierarchy of material microstructure, with length scales ranging from the nanoscale (e.g., small precipitates, dislocations, interfaces) to the microscale (e.g., large precipitates, dislocation cell substructure) and above (e.g., arrangement of phases and grains).<sup>45</sup> As we have seen, Ni-based superalloys are an outstanding example. Within the mesoscale regime alone, their microstructures involve three length scales: (1) the subgrain scale, including the size/shape of  $\gamma'$  precipitates and their spacing within the  $\gamma$  matrix; (2) the grain scale, such as the size and crystallographic orientations of grains; and (3) the polycrystal scale concerning how grains are aggregated.<sup>46</sup> Other families of high-performance alloys bearing such complex, multiphase microstructures include Co-based superalloys, Al-Cu alloys, Mg-Ca-Zn alloys, and twinning-induced and transformation-induced plasticity steels.<sup>7,20,47,48</sup>

Many MMMs for the plastic deformation response of polycrystalline alloys employ plastic crystal plasticity (CP) theory. CP theory relates the distortions of a strained crystal to slip on crystallographic slip systems. Ideal for microstructure-sensitive calculations in alloys are combinations of CP with 3D full-field, spatially resolved mechanics techniques, such as CP finite element (CPFE) or CP fast Fourier transform (CP-FFT) solvers. To date, these MMMs have been advanced so that they span a wide range of scales, from nonuniform, time-varying applied fields (such as in mechanical shaping processes) to the sample, the multiphase microstructure at the meso-scale, granular features such as texture and grain size within each phase at the microscale, and the crystal structure and associated operation of slip and twinning at the nanoscale. They explicitly couple the effects of microstructure morphology and crystallinity in the calculation of stress and strain evolution inside the grains and at the boundaries and interfaces.

Application of CPFE-based modeling for Ni-based superalloys, including multiscale microstructures, can be found in many recent works.<sup>49,50</sup> Keshavarz and Ghosh<sup>46</sup> developed a two-scale CPFE model to incorporate three mesoscale microstructures (**Figure 6**). At the subgrain scale, mechanistic processes, such as dislocation evolution with non-Schmid effects and temperature dependence, APB shearing of  $\gamma'$  precipitates, and microtwinning, have been taken into account. (Non-Schmid



**Figure 5.** (a) Effect of alloying addition on tension-compression (T–C) yield stress ratio for magnesium alloys. Magnesium alloys with different alloying elements are characterized by the plastic anisotropic (PA) measure. (b, c) Polycrystal yield surface ( $\pi$ -plane projection) for different magnesium alloys at 3% compressive strain along the rolling direction.<sup>37</sup> (b) The Mg4Li alloy has one of the smallest PA measures, showing low tension-compression yield stress asymmetry; (c) the ZW41 alloy has the largest PA measure and concomitantly large tension-compression asymmetry.



effects mean that dislocation slips are not initialized on slip planes with the largest resolved shear stress.) At the grain and polycrystal scales, they introduced an activation energy (AE)-based CP model that homogenized subgrain scale responses; a model for geometrically necessary dislocations was also developed. The MMM was able to reproduce the tension-compression asymmetry and temperature-dependent change in the type of slip mode that dominates, an unusual characteristic of these alloys that had been a challenge to predict.

### Grain neighborhood effects in alloys that twin

Challenges remain in designing structural hcp alloys since they can potentially deform not only by slip, but also by deformation twinning. Deformation twinning is receiving a lot of attention, since it is not as well understood as plastic slip, and has a stronger effect on the mechanical response when it occurs.<sup>51</sup> When the alloy is strained, atomic-scale twins can form inside grains or grain boundaries and grow a few orders of magnitude to span the grain. The twin domain abruptly reorients and shears the lattice.

Alloying greatly affects the propensity of twinning and plays a significant role in the twin architecture that develops with straining. Twins that transmit across grain boundaries can detrimentally lead to the formation of “twin chains” percolating across the sample and triggering fatigue cracks

and premature failure.<sup>52–54</sup> Twins that instead remain in their parent grain and multiply in the form of 3D intersecting networks can favorably lead to simultaneous high-strength and large-compression strain to failure.<sup>55</sup> How alloying controls twin development is largely unknown.

In the last few years, multiscale modeling tools for discrete twin domains in this meso-scale regime have been developed.<sup>56–59</sup> These techniques enable calculations of the local stress fields and dislocation activity around twin lamellae, shedding light on the effects of size and local grain neighborhoods on the propensity for twin growth. In one study, this type of multiscale model based on CP-FFT was employed to study the effect of alloying on the transmission of twins across grain boundaries.<sup>60</sup>

**Figure 7a–b** plots the ratio of a driving force for transmission into the neighboring crystal across the boundary to that for growth of the same twin in its own parent crystal with respect to the misorientation of the neighboring grain. Two Mg alloys, AZ31 and Mg4Li, are considered, and in both, the driving force ratio rapidly decreases from unity at zero misorientation (no grain boundary) to zero as the misorientation between the two crystals increases, a trend that would be expected from purely geometric arguments. The important finding is the strong influence of alloying on the cut-

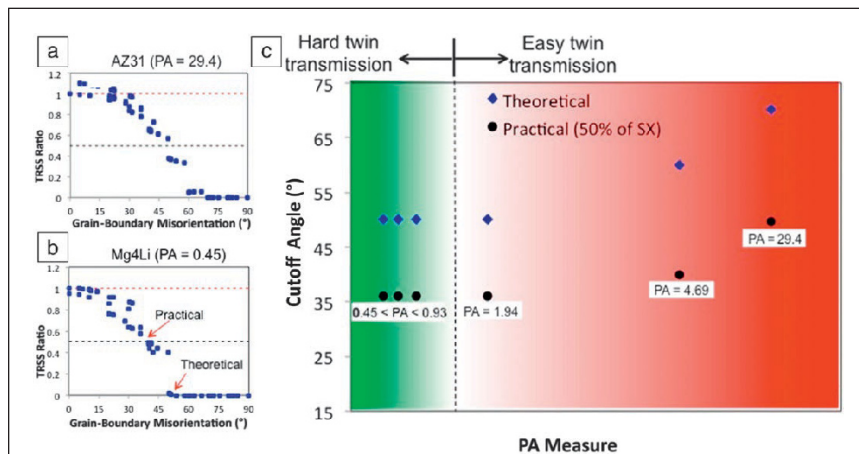
off misorientation angle,  $\Delta\theta_{\text{cut}}$ , above which the driving force and chances for twin transmission are zero. The alloy with the higher PA (Equation 1), AZ31, has a much higher  $\Delta\theta_{\text{cut}}$  than Mg4Li, with the lower PA. Evidently, alloys with larger CRSS gaps among their slip modes promote twin transmission.

Figure 7c maps the calculated  $\Delta\theta_{\text{cut}}$  for a wide range of Mg alloys. For more anisotropic (higher PA) alloys,  $\Delta\theta_{\text{cut}}$  increases with PA, while for lower PA alloys,  $\Delta\theta_{\text{cut}}$  is fixed at a lower value of  $\sim 50^\circ$ . These multiscale CP-FFT predictions reveal that alloying can have a more direct effect on twin morphologies than first thought. This insight suggests that alloying can help prevent twin chains from forming and acting as preferred paths for shear banding or cracking.

### Opportunities and challenges

As we have highlighted, significant advances have been made in linking composition, microstructure, and mechanisms with the development of local stress states and deformation response. Yet several multiscale modeling challenges remain in the quest to fully understand the processing–microstructure–response relationships of an alloy.

During deformation, particularly under elevated temperatures and over long periods of time, a number of phenomena can occur that involve stress-induced migration of internal boundaries, such as phase transformations, recrystallization,



**Figure 7.** Variation of the driving force for twin transmission across a grain boundary with the misorientation of the grain boundary for two Mg alloys (a) AZ31 and (b) Mg4Li. A value of unity implies that the driving force for twinning in the neighboring grain at the tip of the twin is equal to that for twin propagation of the same twin in its parent crystal. A high (or too high) misorientation regime is well marked by a cutoff misorientation angle  $\Delta\theta_{\text{cut}}$ , above which the chances for twin transmission are zero. (c) Map of the variation of cutoff angles for a wide range of alloys. Alloys are indicated by their plastic anisotropic (PA) measure in Equation 1. An arbitrarily defined practical cutoff angle, associated with a driving force ratio of 0.5 is also marked. This angle corresponds to a neighboring grain that bears a driving force that is 50% lower than that to propagate a twin in its own parent crystal. These more practical cutoff angles follow the same variation with PA as seen in (c). However, this 50% chance misorientation angle is more likely to be consistent with experimental observation. It is reasonable to expect that twin transmission would rarely be seen, particularly when the data sets are small, for misorientations corresponding to this practical cutoff angle, which is  $\sim 36^\circ$  for the low PA alloys and  $\sim 50^\circ$  for the highest one.<sup>60</sup>

grain growth, crack growth, and deformation twins. Many of these aspects have been studied intensively using atomic-scale simulations and phase-field methods, but incorporating their effects into slip and twinning in MMM codes has been challenging. Recent advances in this area have involved concurrently combining phase-field and CP theory into a single simulation tool, allowing for updates of crystalline and thermodynamic properties of the phases, lattice defects, and kinetics of migrating interfaces in time or strain.<sup>61–63</sup> These have been used to understand the influence of dislocation dynamics on rafting and how microstructural evolution can constrain or facilitate dislocation activity.

Many newly developed ultrastrong alloys have a highly heterogeneous grain structure. Some microstructural regions consist of micron-sized grains, while other regions are nanostructured, comprised of nanotwins, bimetal nanolayers, metal-ceramic nanolaminates, and nanograins.<sup>64,65</sup> No model to date can treat the plasticity in a such a significantly varied grain structure. Current multiscale models treat plasticity in coarse grains by using scale-independent, statistical dislocation densities over long time scales, and in nanograins by the scale-dependent motion of discrete dislocations over short time scales. New methodologies that can address discrete slip occurring over long times, in which microstructural evolution can be captured, are needed to design newer forms of heterogeneous alloys. Some recent advances to implement discrete slip events into a CPFE framework have been applied

to relatively simple single-phase, pure metal systems.<sup>66</sup>

Many high-performance alloys are multi-phase, wherein more than one phase can plastically deform. Atomic-scale simulation and *in situ* microscopy of deforming groups of grains have revealed a number of defect–interface reactions (transference, recovery, nucleation) that could significantly affect the types of slip and twinning modes that would be selected in deformation.<sup>67,68</sup> Representing the role of such highly resolved atomic-scale reactions into the local orientation of crystals and ultimately the mechanical response is beyond current modeling capabilities. To benefit from advancements in alloys by microstructure design and control, MMM extensions toward incorporating the role of dislocation/interface interactions is recommended.

## Outlook

Overcoming the “mesoscale gap” is rapidly becoming an MMM community-level effort. Notable research-center-level efforts exist that have successfully connected methodologies that span the broad atoms-to-continuum time scale and length scale spectrum.<sup>69,70</sup> Data I/O, codes, and reports are increasingly being

shared in repositories, publications, and public websites and hubs worldwide.<sup>71,72</sup> In tandem are growing efforts to train users, via online manuals, example cases, summer schools, and workshops.<sup>73,74</sup> Leaps in computing power are undeniably indispensable to fully develop and realize the predictive capabilities of many MMMs. Promising ways toward enabling larger and longer time simulations include adopting novel computing architectures, innovating efficient computational schemes, and using government and national laboratory facilities such as the High Performance Computing facilities,<sup>75–78</sup> and the US Department of Energy’s Exascale Project.<sup>79</sup> The Minerals, Metals & Materials Society recently published two reports, *Modeling Across Scales*<sup>80</sup> and *Core Knowledge and Skills*,<sup>81</sup> to inform the public of methodology and knowledge gaps. By coming together, MMMs for alloys can truly conquer the length scales within our lifetime.

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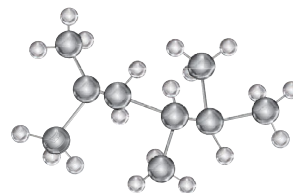


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