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Concepts on Low Temperature Mechanical Grain Growth

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Concepts on Low Temperature Mechanical Grain Growth

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Abstract

In metals, as grain size is reduced below 100nm, conventional dislocation plasticity is suppressed resulting in improvements in strength, hardness, and wears resistance. Existing and emerging components use fine grained metals for these beneficial attributes. However, these benefits can be lost in service if the grains undergo growth during the component's lifespan. While grain growth is traditionally viewed as a purely thermal process that requires elevated temperature exposure, recent evidence shows that some metals, especially those with nanocrystalline grain structure, can undergo grain growth even at room temperature or below due to mechanical loading. This report has been assembled to survey the key concepts regarding how mechanical loads can drive grain coarsening at room temperature and below. Topics outlined include the atomic level mechanisms that facilitate grain growth, grain boundary mobility, and the impact of boundary structure, loading scheme, and temperature.

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NOMENCLATURE

BCC	Body-centered Cubic
CSL	Coincident Site Lattice
DSC	Displacement Shift Complete
DOE	Department of Energy
FCC	Face-centered Cubic
GB	Grain Boundary
MD	Molecular Dynamics
SMiG	Shear Migration Geometrical Model
SNL	Sandia National Laboratories
TEM	Transmission Electron Microscopy

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1. INTRODUCTION, WHAT IS MECHANICAL GRAIN GROWTH?

Most scientists first learn of grain growth as a thermal process governed by Arrhenius kinetics associated with diffusion. At the atomic scale, visions are conjured of individual atoms "hopping" one-by-one across a grain boundary by slightly adjusting their lattice position to associate with the growing grain's lattice at the expense of the shrinking grain. While the thermal process for grain growth is certainly the most technologically important, it is possible to drive grain growth through mechanical means. Mechanical grain growth can be defined as the coarsening of a grain structure that is caused by or accelerated by mechanical stresses or strains.

To begin, consider the various ways mechanical loads can interact with a grain structure to initiate grain growth. In 1949, Beck and Sperry [1] observed coarsening in high purity aluminum that was heated after being previously plastically deformed. The growth occurred through the motion of grain boundaries (GBs) that would consume grains with high dislocation density replacing the region with a pristine lattice (Figure 1a). What was particularly peculiar about their observation was that a nearly flat, low-curvature boundary evolved into a macroscopically tortuous boundary of considerably higher surface area, precisely opposite to the thermally-driven process where curvature is reduced to minimize boundary area and hence boundary free energy. The migration was determined to be "motivated by excess free energy from strain hardening." In other words, the differences in plastic strain energy between grains initiated boundary motion to consume crystals with high dislocation content. Beck and Sperry's observation of defect-driven GB migration is reminiscent of recrystallization [2], an "annealing" process occurring by the nucleation and growth of defect free grains either after or during straining i.e. dynamic recrystallization [3].

In addition to dislocation content associated with plastic strain, stresses are also known to initiate GB motion resulting in coarsening. In 1954, Bainbridge et al. sheared Zn [4] at, above, and below room temperature. At all three temperatures, GB motion in response to the applied load was observed. An example of boundary motion at 375°C is provided in Figure 1b. Stress can drive GB motion through two paths. The first possibility is GB motion from differences in elastic energy associated with crystallographic stiffness anisotropy. The second path is a direct interaction of the mechanical load with the interface. A GB is essentially comprised of defect clusters whose atoms can be "pushed" by a stress field to induce motion. This scenario is akin to shear stresses causing the glide of a dislocation array.

In some instances, the mechanical loading does not directly drive coarsening but accelerates traditional thermal growth mechanisms. Strain enhanced coarsening of solder is one such example. In service, solder joints undergo thermo-mechanical fatigue due to mismatch in thermal expansion coefficients of the solder with its substrate. Local coarsening as discussed in [5], has been found to occur along the direction of shear strain and Frear et al. propose that the strain creates voids and dislocations to accelerate diffusion based coarsening [6].

From the above examples, it is seen that grain growth has traditionally been studied with elevated temperature which may lead one to think that coarsening does not readily occur in the low temperature regimes. It is worth reiterating however that Bainbridge et al. [4] observed mechanical growth at room temperature and at cryogenic temperature. A significant number of other low temperature mechanical growth examples, especially in nanocrystalline materials, have been reported [7-15] from both experiments and simulations. A vivid example of this is shown in

Figure 1c where *in situ* TEM tensile loading of nanocrystalline Al at room temperature results in GB migration [16]. Overall, these findings suggest that mechanical coarsening may occur through processes that do not necessarily require elevated temperatures. This notion is perhaps counter intuitive considering that low temperatures are customarily used to "lock in" a grain structure as with quenching. This work focuses on the novel or less traditional low temperature mechanical grain growth. While parallels will be drawn to high temperature observations, in this brief review we will show that there are well-established thermodynamic driving forces at low temperature and address how GBs have sufficient mobility at low temperatures to facilitate mechanical grain growth.

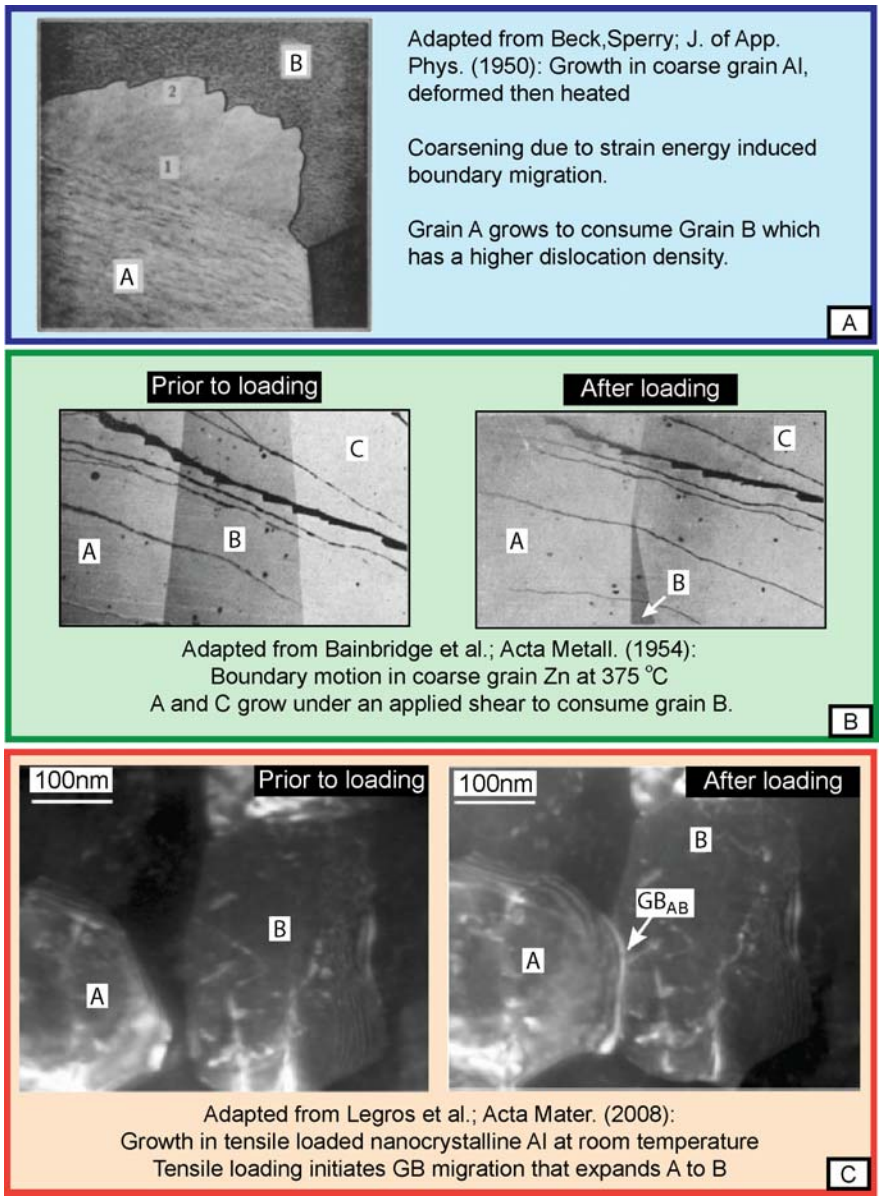

Figure 1: Examples of mechanical coarsening via GB migration by plastic strain (a), elastic stress (b), and tensile loading (c)

2. PHENOMENOLOGY OF MECHANICALLY DRIVEN GRAIN BOUNDARY MOTION

Mechanically induced grain growth occurs either through GB motion normal to the boundary plane where the moving interface consumes neighboring grains while coarsening the parent grain, or by grain rotation with tangential boundary motion along the boundary plane (sliding) resulting in the merging of two grains into coincident crystallographic alignment. Both of these processes are discontinuous in the sense that grains grow at the expense of neighbors as opposed to all grains coarsening in a normal fashion. For the former case i.e. no sliding, the motion of a boundary is commonly expressed as a product of driving force and mobility as given in Equation 1

Equation 1: Expression for the velocity of a moving GB

$$v = m \cdot p$$

where v [m/sec] is the velocity of the GB, m is the mobility [m/Pa-sec], and p [Pa] is the driving force (note that it is common convention to express the driving force in units of Pascals instead of Newtons). Therefore to describe GB migration, one must comprehend the details behind both the driving force term and the mobility term.

2.1 Driving Forces

There are three main mechanical driving forces namely, elastic strain energy, plastic strain energy, and applied stress. The elastic strain driving force arises from the energy difference between grains due to differences in stiffness from crystallographic orientation. The extent of this driving force will thus be governed by the material's degree of anisotropy. Elastic strain energy can be computed as a sum of the product of the stress and strain tensors, $\frac{1}{2}\sigma_{ij}\varepsilon_{kl}$. For elasticity, $\sigma_{ij} = C_{ijkl}\varepsilon_{kl}$ with C being the elastic stiffness tensor. Indicial notion has been used to show that C has 81 terms, 21 of which are independent due to the symmetry of C, σ, and ε. C can be further simplified by the crystal structure symmetry (cubic, hexagonal, tetragonal, etc…) of the particular material in question. Thus for any two neighboring grains, the driving force can be estimated using Equation 2.

Equation 2: Elastic energy driving force

$$p = \left[0.5 C_{ijkl}\varepsilon_{ij}\varepsilon_{kl}\right]_{Grain\ 1} - \left[0.5 C_{ijkl}\varepsilon_{ij}\varepsilon_{kl}\right]_{Grain\ 2}$$

The plastic energy driving force stems from differences in dislocation density content amongst the grains and can be expressed using Equation 3.

Equation 3: Plastic strain energy (stored deformation) driving force

$$p = \frac{1}{2}(\Delta\rho)\mu b^2$$

where $\Delta\rho$ is the difference in dislocation density between two grains, μ is the shear modulus, and b is the length/magnitude of the Burgers vector. The force from stored deformation energy will be dependent on the active deformation mechanism of the material. For coarse grained and microcrystalline metals whose plasticity results in considerable dislocation storage this driving

force will be central. However for nanocrystalline metals, with smaller grains holding less dislocation content, this driving force is expected to have minor impact.

The third driving force is the applied load causing direct motion of a boundary. This force, expressed as the shear stress on the boundary, drives motion through processes detailed in section 2.2.

Equation 4 formally expresses the stress driving force as

Equation 4: Applied stress driving force

$$p = \beta\tau$$

where τ is the shear resolved on the interface. The term, β, as described by Cahn et al. [17, 18] depends the structure of the GB and is thus a geometric factor linking shear tangential to the GB to boundary motion normal to the interface.

Discounting diffusion based driving forces as discussed in [19-21], there are still non-mechanical factors, creating free energy differences between grains, to provide additional driving force for growth. Such factors include GB curvature [22] as well as gradients from magnetic fields [23-25]. For homogenous systems free from strong electro-magnetic fields, the magnetic force contributions will be negligible. The curvature force however inversely scales with grain size thus augmenting the forces available for the coarsening of nanocrystalline systems.

In [26], Gottstein estimates the magnitude of various driving forces from free energy differences amongst the grains of a material. For coarse grained homogenous systems, the forces are relatively weak with plastic strain (stored deformation) driving force being on the order of 10 MPa and elastic stress driving force only on the order of 2.5 x 10^{-4} MPa. These seemingly low values may stem from the fact that Gottstein's estimates are for materials at elevated temperatures. In this regime, the free energy change of an atom going from the shrinking grain to the growing grain will be much less than the thermal energy. His observation is drawn by considering Al at 723 K with a strain energy driving force of 10 MPa where $p_v n^3/kT$ equals 0.01. In this comparison, the driving force energy is $p_v n^3$ where p_v is the driving force from free energy differences and n^3 is the volume of a single atom (~2.7 x 10^{-29} m^3). The thermal energy is kT where k is Boltzmann's constant (k = 1.381 x 10^{-23} J-K^{-1}) and T is absolute temperature. Since strain energy driving force is small it remains to be seen if applied stress is sufficient to induce GB motion. Models by Gutkin et al. [27] and Dynkin et al.[28] estimate GB migration can initiate at shear stress levels of tens to hundreds of MPa range, reasonable for high strength nanocrystalline systems.

Consider adapting Gottstein's "back of the envelope" calculation regarding energy to compare statistical motion of a GB due to temperature with the work done by an applied mechanical load in moving a GB. The total energy of the system can be expressed as

Equation 5: Total energy available to drive GB motion

$$E_{total} = E_{Drive\ Force} + E_{Thermal}$$

with

Equation 6: Expression for thermal energy

$$E_{Thermal} = kT$$

and

Equation 7: Expression for energy associated with applied shear stress and any other driving force such as curvature.

$$E_{Drive\ Force} = (p_v + \tau\beta)n^3$$

Equation 7 was constructed following Cahn's outline [17] and p_v is the free energy driving force, τ is shear stress, and β is the coupling/scaling factor. Estimates using nominal values from published experimental studies are provided in Table 1. The data comes from two types of specimens: bi-crystal or large grain samples that were sheared and nanocrystalline foils that were indented or axially loaded. In constructing Table 1, it was necessary to make approximations for some variables, particularly the shear stress resolved on the boundary (τ), the coupling factor (β) and the free energy driving force (p_v).

For bi-crystal specimens, it was possible, to estimate the shear stress operating on the GB and the coupling factor. However for cases of axial loaded nanocrystalline material, a crude back-of-the-envelope estimate could be calculated based on the following assumptions. The GB in question is assumed to be under the worst-case scenario: inclined at 45° relative to the loading axis so that the maximum shear stress, e.g. one half of the axial stress, is resolved on the GB. If indentation is employed to drive GB migration, the Tabor relation is used to extract the yield stress from the hardness (Hardness = 2.9 x Yield) and then half the yield stress is taken as the shear resolved on the boundary. Concerning the coupling factor (β), a value of 0.5 is assumed.

For the free energy driving forces, if the material is nanocrystalline, then grains are assumed too small to accommodate dislocations (no strain energy driving force) but a curvature driving force from the GB will assist the applied load. Curvature driving force is $p_v = 2\Upsilon/R$ where Υ is the GB energy taken to be 0.5 J/m^2 which was assumed by Gottstein [26] and is in line with GB energy calculations for Al [29, 30]. R is the radius of the grain taken to be spherical in shape. No free energy driving forces are assumed for the coarse grain specimens as these were typically sheared with elastic loads and would not have differences in plastic strain energy. Also due to the large grain size, the curvature would provide minute assistance to the driving force. Lastly, all other driving forces are assumed to be negligible (magnetic, chemical, elastic anisotropy, etc…).

Table 1: Estimate of energy available to drive GB motion from published experimental data

Reference	Mechanical Driving Force, τβ (MPa) [estimated shear stress on GB, MPa]	Curvature Driving Force (MPa) [Grain Size, nm]	Sum of Mechanical & Curvature Energy, eq. 7 (J)	Temperature (K) [$T_{homologous}$]	Thermal Energy (J)	Total Energy (J)
Al, tension [9]	37.3 [74.5]	22.2 [90]	$1.6x10^{-21}$	298 [0.32]	$4.1x10^{-21}$	$5.7x10^{-21}$
Cu, indentation [8]	172 [345]	44.4 [45]	$5.9x10^{-21}$	77 [0.06]	$1.1x10^{-21}$	$6.9x10^{-21}$
Pt, tension [12]	400 [800]	100 [20]	$1.4x10^{-20}$	298 [0.15]	$4.1x10^{-21}$	$1.8x10^{-20}$
Ni, compression [13]	500 [1000]	100 [20]	$1.6x10^{-20}$	298 [0.17]	$4.1x10^{-21}$	$2.03x10^{-20}$
Co-P, tension [10]	488 [975]	167 [12]	$1.8x10^{-20}$	298 [0.17]	$4.1x10^{-21}$	$2.2x10^{-20}$
Al, shear [31]	0.02-0.1 [0.1-0.5]	0 [bi-crystal]	$4.3x10^{-25}$ – $2.8x10^{-24}$	593 [0.64]	$8.19x10^{-21}$	$8.19x10^{-21}$
Al, shear [31]	0.02-0.08 [0.02-0.08]	0 [bi-crystal]	$4.3x10^{-25}$ – $2.2x10^{-24}$	593 [0.64]	$8.19x10^{-21}$	$8.19x10^{-21}$
Zn, shear [4]	0.003-0.004 [0.003-0.004]	0 [coarse grain]	$8.9x10^{-26}$ – $1.1x10^{-24}$	77 [0.11]	$1.1x10^{-21}$	$1.1x10^{-21}$
Zn, shear [4]	0.002-0.003 [0.002-0.003]	0 [coarse grain]	$4.7x10^{-26}$ – $8.5x10^{-26}$	573 - 673 [0.83 - 0.97]	$7.9x10^{-21}$ – $9.3x10^{-21}$	$7.9x10^{-21}$ – $9.3x10^{-21}$

Three observations are made from the data compiled in Table 1. The first is that for the nanocrystalline materials loaded at low temperatures, the energy from the mechanical driving force energy approaches and in several cases exceeds the thermal energy. The applied loads are indeed reasonably attainable so the work done on the GB through stress provides the energy needed for GB motion not fulfilled by the thermal energy. The second is that the Zn experiments by Bainbridge et al. [4] demonstrate that GB motion is highly sensitive to the applied load. For the Zn, even at 77 K, the thermal energy of the system overshadows the driving force energy. This may seem anomalous, however, one must keep in mind that the Zn experiments involve the motion of a very specific type of boundary and loading condition. Bainbridge et al. studied flat, low angle GBs (~1° misorientation) with shear applied in the direction of the Burgers vector of the dislocation array that comprises the boundary. The set-up is akin to that represented in Figure 2. The data reveal that a driving force energy approximately four orders of magnitude less than the thermal energy is sufficient to start the coarsening process. The final observation is that as an overall trend, GB migration is active so long as the total energy of the system is above ~1 x 10^{-21} J. This notion is also corroborated by Gerth et al. [32] who tabulates the driving forces for Al-1% Si under thermo-mechanical stress. If the driving force data in [32] is converted into units of Joules with the n^3 term from Equation 7, then the total energy is in general agreement with the values of Table 1. Altogether, it may be that the focus on individual energy levels whether mechanical or thermal is not as critical as the total energy of the system available to drive GB migration.

2.2 Atomic Processes for Grain Boundary Migration

Many of the early theories for GB migration are centered on the thermally activated transport of single or multiple atoms from one grain to another. Gleiter [33] theorized GB migration to occur through a diffusive process where individual atoms detach from a kink or ledge on the shrinking grain, diffuse through the GB, and then attach to a newly created lattice site on the growing grain. Mott [34] proposed that the process could be multi-atom based where clusters at an interface can disorder or partially melt and then re-solidify to match the structure of the growing grain. Experimental insights suggest GB motion is indeed a multi-atom process. High resolution electron microscopy of Au bi-crystals by Merkle et al. [35, 36] observed GB motion to occur through groups of atoms rearranging at the interface in a cooperative fashion. What types of multi atom mechanisms then facilitate GB motion, especially at low temperature where long range diffusion is expected to be subdued?

The motion of a GB at low temperatures can be understood from models that represent an interface with dislocations. Read and Shockley [37] modeled GBs using dislocation arrays and this approach works beautifully as edges and screws can be configured to represent tilt and twist interfaces at less than ~15° of misorientation. With this model, it can be seen that an applied load develops shear stresses causing the collective glide of the dislocation array, i.e. the grain boundary [38]. This concept is illustrated in Figure 2.

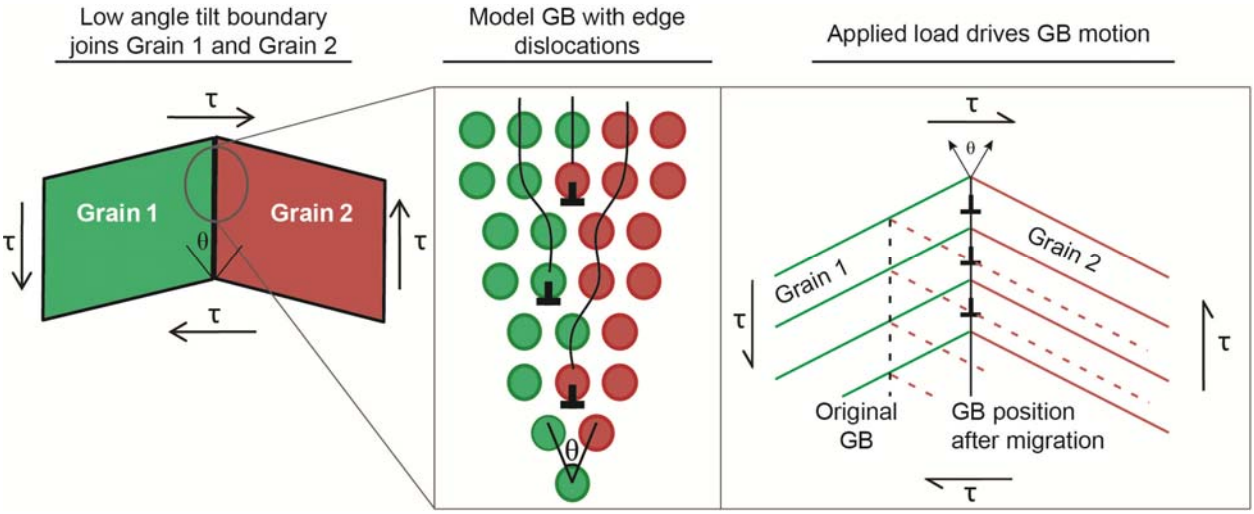

Figure 2: Schematic showing the migration of a low angle tilt boundary modeled as an array of edge dislocations. Figure adapted from Molodov et al.; Acta Mater. (2007).

This simple approach demonstrates how mechanical loads can drive boundary motion at low temperatures however two issues exist. The first is that a difficulty arises when attempting to understand how mechanical loads interact with high angle grain boundaries. At large misorientations, the spacing between the dislocations in the Read and Shockley model has to be reduced so much that the dislocations would overlap and lose physical meaning. The second complication is that the passage of dislocations at a boundary will require the grains to deform/shear relative to each other. In polycrystalline systems, grains may be constrained in such a fashion that requires GB motion without shear. The following paragraphs review a summary by Caillard et al. from [39] that outlines the various GB migration models that can operate with and without shear.

For situations when shearing and long range diffusion are prohibited, Rae et al. [40] suggest that GB motion may be possible through short range diffusion or by passing a particular set of dislocations whose Burgers vectors sum to zero but the step heights do not. In [41], Babcock and Balluffi studied near Σ5 boundaries in Au and observed instances migration without noticeable dislocation activity. To explain such boundary migration, the authors propose that at the interface, groups of atoms are undergoing a conservative shuffling with possible assistance from local diffusion. With the GB motion due to local rearrangements and shifting of atoms, this mechanism is essentially applicable to all boundary types. Simulations have also provided support for this mechanism. Babcock makes a direct link to shuffling seen in simulations of a Σ5 twist boundaries [42] and a similar shuffling mode has been reported in other simulations as well [43, 44].

For cases when deformation or shearing of grains is free to occur, several models have been proposed. Rae et al. analyze the motion of GBs as being facilitated through the displacement shift complete (DSC) model [40]. For this model, boundaries that follow the coincident site lattice relationship can be described with a DSC lattice that encompasses both crystallites on either side of the boundary. Mechanically driven motion of DSC dislocations can thus lead to the migration of the interface. This mechanism has been identified experimentally in Al by Fukutomi et al. [45, 46] and also reported by Babcock and Balluffi [47]. While this mechanism can explain the motion of high angle GBs, its applicability may be limited to interfaces that meet the requirement for the coincident site lattice relationship.

Cahn and Taylor [17] proposed a unified approach to the motion of GBs centered on a shear coupled mechanism developed by analyzing symmetric tilt and twist boundaries. They state that the motion of a grain parallel to an applied shear ($v_{||}$) can couple to a GB inducing its motion normal to that shear (v_n). These two motions are linked by a geometric coupling factor, β, where $v_{||} = \beta\, v_n$. This purely mechanical GB motion is therefore centered on the coupling factor, β, which is determined from the dislocation content of the interface [48]. While not immediately intuitive, Cahn uses the dislocation description of the GB to determine β for both low and high misorientation scenarios. For low angle boundaries, the coupled motion will be akin to that described in Figure 2 and this shear coupling through β has been confirmed experimentally as reported in [31]. For high angle GBs, molecular dynamics (MD) simulations [18, 49, 50] confirmed the validity of still using β and provided insights to the atomic level activities facilitating the GB motion. The simulations reveal that the interface can be organized into repeating structural units or clusters of atoms that Cahn calls “kites”. The applied mechanical load can then induce the collective shuffling and rotation of the kites resulting in a translation of the boundary. This process, as sketched in Figure 3 for a high angle ∑17 coincident site lattice (CSL) boundary, has not only been observed in the Cahn-Mishin simulations but in simulations of 3D grain boundary networks [51] by Velasco as well.

Experimentally, the theoretical coupling factor, β has been shown to be apt in describing the motion of high angle symmetric tilt boundaries in Al bi-crystals [52, 53] as well as mixed GBs with both tilt and twist components [54]. However as Molodov et al. [55] found, the coupling factor can deviate from Cahn’s theoretical value when the interface becomes asymmetric. This deviation appears to be due to Cahn’s model being constructed around the analysis of symmetric boundaries.

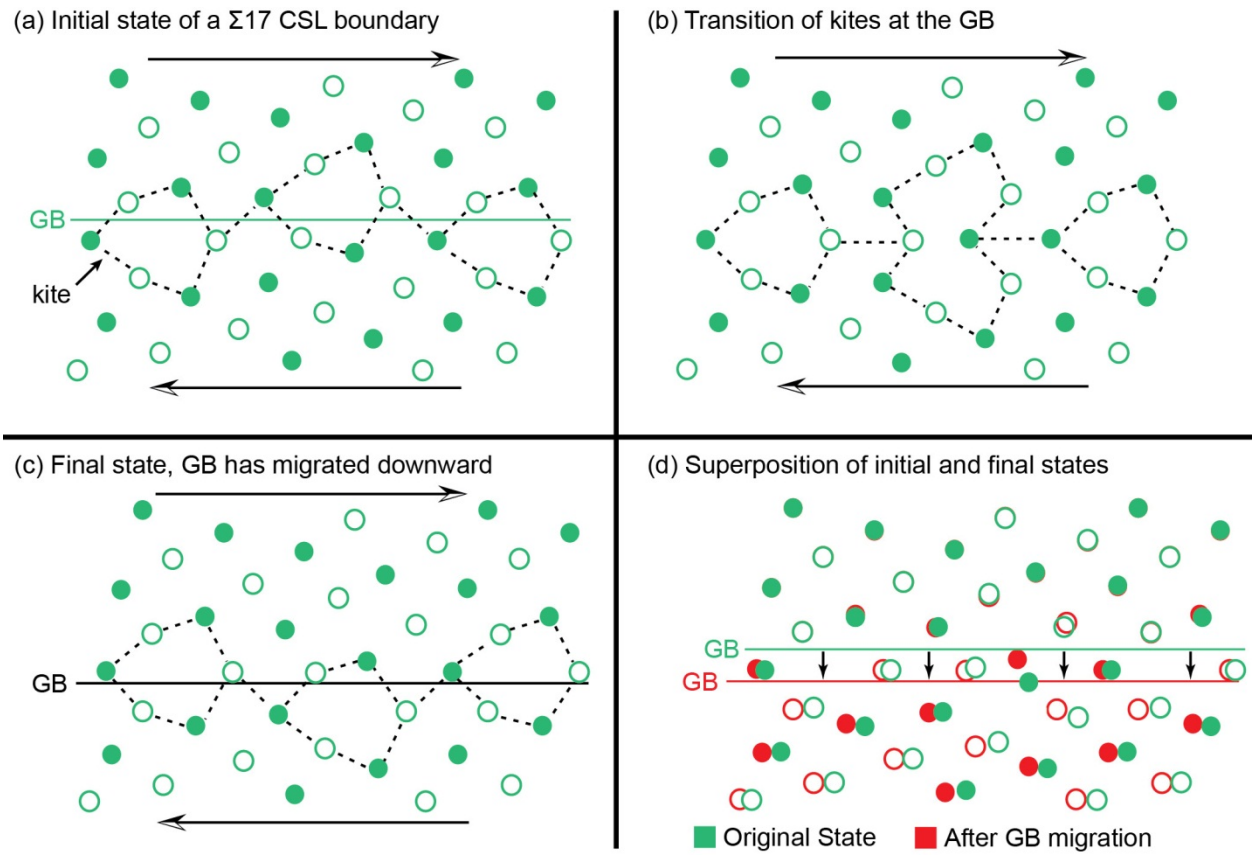

Figure 3: Schematic of the atomic level activity that results in the motion of a high angle CSL GB. The original interface is shown in (a) with the intermediate state where atoms at the boundary shuffle and rotate in (b) and the final state shown in (c). The superposition of the initial and final states is shown in (d). Figure adapted from Cahn et al.; Acta Mater (2006).

As the majority of GBs in a polycrystalline system are expected to have a more "general" structure, Caillard et al. have ventured to develop a generic model applicable to any interface configuration. With their two part study [39, 56], using *in situ* TEM techniques, mechanically driven GB motion in Al was studied and used to develop the Shear Migration Geometrical Model (SMiG) that can explain the motion of general boundaries. The model is purely geometric and the shear coupling again occurs via local atomic rearrangement without any long range diffusion. The process can be thought of as finding a rotation and shear path that will transform one grain's lattice to match its neighbor. The coupling factor β can then be determined from the geometry of the transformation. Caillard and colleagues continue to develop the SMiG approach and have demonstrated its application to a more general spectrum of GBs [57, 58]. Most recently, experiments and simulations from this group [59, 60] suggest the unit level mechanisms of shear coupled GB motion to be driven by the nucleation and motion of GB steps that are linked to disconnections [61] which have been noted by others [62, 63] as well.

One other mechanism to consider is that of Gutkin and Bobylev [27, 64, 65] who analyze boundary motion using rotational defects or disclinations. Due to an applied load, stress building up at the junction of GBs can form disclinations whose motion subsequently facilitates GB migration. If one steps back and considers disclinations as Romanov [66] does with "the generation and motion of disclinations is the collective effect of dislocation ensembles" then this

mechanism also has roots in the mechanical load causing clusters of atoms at the boundary to shift and rotate. While the exact details of mechanically driven GB motion are still being developed, all models mentioned above share a common thread in that the GB migration occurs through the motion of clusters of atoms at the interface.

2.3 Boundary Mobility

The mobility term of Equation 1 must also be addressed. The mobility of a GB is effectively a measure describing how easy it is to move the interface. This term is of interest as more mobile boundaries will be easier to move and thus be the ones active during the mechanical growth process. Historically, mobility has been considered to follow Arrhenius type temperature dependence as expressed in Equation 8

Equation 8: Expression for GB mobility

$$m = m_o \exp\left(\frac{-E}{kT}\right)$$

where m_o is a pre factor, E is the activation energy for boundary motion, k is Boltzmann's constant, and T is absolute temperature. This definition works well for classic mobility studies [67] and matches the traditional thermally activated description of GB motion. However an issue is that this relation would predict low or near zero mobility for GB migration at lower temperatures. This contradicts room temperature *in situ* TEM observations of fast GB motion in nanocrystalline Al [11, 16] where GB velocities of up to 200 nm/sec were reported by Legros et al. For perspective, consider Winning's study on the stress driven migration of <100> Al tilt boundaries [68] at 700 K. For the high misorientation interface, the activation energy was determined to be $E = 1.2 \times 10^{-19}$ J with a pre factor of $m_o = 0.83$ $ms^{-1}MPa^{-1}$ resulting in a mobility of $m = 3.4 \times 10^{-6}$ $ms^{-1}MPa^{-1}$. If a load is applied such that the driving force is 10^{-2} MPa, then the GB should move at a velocity of 34 nm/sec. If the temperature is reduced to 298 K, the mobility of the same GB would drop several orders of magnitude to $m = 1.8 \times 10^{-13}$ $ms^{-1}MPa^{-1}$. At that temperature, to maintain the same velocity of ~34 nm/sec, the driving force would need to exceed 100 GPa, an unrealistic value even for high strength nanocrystalline materials. While the nature of the GBs in the TEM studies are unknown, it is clear that at low temperatures there is disconnect between observed room temperature GB velocities and the Arrhenius temperature dependence of mobility.

Experimentally, GB mobility is typically measured on bi-crystals to avoid confounding effects of triple junctions [69, 70] and adjacent boundaries. Even in ideal bi-crystals, GB mobility is difficult to measure as it is a function of the GB structure specified by five macroscopic parameters [38]. Three parameters specify the lattice rotation between neighboring grains and the remaining two parameters define the plane of the GB. Knowing all five parameters restricts investigations to well defined systems for which only a limited number of boundary configurations can be grown. Gottstein [26] echoes this notion by saying, "in the majority of investigations grain boundary migration was considered for a very few specific boundaries and provide only an incomplete characteristic of the migration capability of grain boundaries." Therefore, not enough experimental information exists to provide a comprehensive characterization of mobility.

With advances in computational methods however, a larger range of GBs can be studied providing new insights. In [71], Olmsted et al. made some particularly interesting observations

that suggest mobility is not always thermally activated. The study computed the mobility of 388 different GB configurations in nickel including tilt, twist, mixed, high, and low angle types. It was found that many of the GBs were thermally activated but surprisingly 117 were not thermally activated ('non-activated'). These non-activated boundaries either had mobility that did not change with temperature (athermal) or had mobility that increased with decreasing temperature (anti-thermal). Furthermore, these non-activated boundaries can be faster in comparison to the thermally activated. Such observations are striking as the non-activated boundaries make up 30% of the studied interfaces; not an insignificant portion. Overall, the simulations suggest that the traditional description, of Arrhenius type behavior, is not complete in describing the mobility of GBs.

Mobility may also be impacted by the driving force. In [72] Halsam et al. use MD simulations to explore the impact of stress on grain growth at elevated temperatures where diffusion is active. The authors find that in the absence of stress, the coarsening is slower. They suggest that in addition to stress being its own driving force, it may also heighten GB mobility and grain rotation mobility to accelerate coarsening. While Equation 1 divides boundary velocity into the product of mobility and driving force, the two terms may not be independent with the mobility being sensitive to driving force. Rough boundaries are faster than slower smooth boundaries and as demonstrated by Olmsted, Holm, and Foiles [73, 74]; GBs have temperatures at which they can change from smooth to rough. This roughening transition can impact the coarsening evolution as fewer smooth interfaces will result in fewer pinning points to stagnate grain growth. Along the same lines, it may be possible for the driving force to cause a kinetic roughening that increases mobility. In this sense, the driving force can transition the GB from smooth to rough in situations where the temperature is insufficient to do so. This roughening may be especially influential during low temperature coarsening where mechanical driving forces are high.

2.4 Stress or Strain Dominant?

The two fundamental consequences of an applied load are stress and strain, but which of these is providing the mechanical driving force for GB migration? Coarsening that occurs through the reduction of dislocation content in large grained metals such as in the experiments by Beck and Sperry [1], demonstrate that the strain (or plastic strain energy) can cause GB migration. However, the driving force is not so clear for nanocrystalline materials. Post deformation TEM analysis of nanocrystalline metals exhibiting grain growth typically shows a lack of dislocation storage. Is stress driving the GB motion without dislocation generation (strain) or is the low dislocation density a result of a recrystallization type mechanism where grains with any appreciable dislocation content are replaced with a strain free lattice? Observations from *in situ* TEM studies do not provide a clear answer. Legros et al. [16] notes that for tensile strained Al films, mechanical coarsening precedes any dislocation activity suggesting the growth is stress driven. On other hand, indention of nanocrystalline Al by Jin et al. [11] resulted in dislocation generation followed by GB motion. Along similar lines, Wang, Li, and colleagues [75, 76] attributed twin boundary motion to the passage of twinning dislocations.

Quantitative evidence exploring this issue is available from experiments by Rupert et al. [77] who deformed nanocrystalline Al films with strategically placed stress concentrators creating distinct regions of maximum stress and maximum strain in the specimen. By measuring the grain size distribution in these regions it was determined that the most grain growth corresponds to regions of maximum stress, particularly shear stress. While this work points

towards the mechanical growth process being most sensitive to shear stress, it does not discount growth due to strain which may operate in parallel to the stress driven process.

3. FACTORS AFFECTING MECHANICAL GRAIN GROWTH

To better understand mechanical grain growth, it is important to elucidate how the intrinsic and extrinsic factors of a material system promote or inhibit coarsening. In this section, the intrinsic factors of GB character, crystal structure, and purity and the extrinsic factors of loading scheme, and temperature, are considered.

3.1 Crystal Structure

While coarsening at elevated temperature has been reported to be active in a variety of crystal structures, mechanical grain growth at low temperatures has been primarily observed in face-centered cubic (FCC) nanocrystalline metals including Al [9, 11, 16], Cu [7, 8, 78], Pt [12, 79], and Ni [13, 80]. A nanocrystalline Co-P system [10] also exhibits mechanical coarsening and while Co is hexagonal, the Co-P system actually has an FCC structure. Mechanical growth in hexagonal systems has been limited to the study on Zn by Bainbridge [4], simulations by Khater et al. [63] and a report on the activity of stress driven coarsening in ultra-fine grain Mg [81]. It remains to be seen if low temperature mechanical growth is widely active in body-centered cubic (BCC) materials. With regards to the proposed atomic level mechanisms (Section 2.2), there are no stipulations or conditions in terms of crystal structure. Although, with the theoretical models rooted in the GB motion being analogous to the glide of dislocations, there may be lattice friction effects similar to that of a Peierls-Nabarro stress. In [18], Cahn remarks that the critical stress for shear coupled GB motion at low temperature ”can be identified with the Peirels-Nabarro stress for the collective glide of the array of parallel straight dislocations”. This suggests that the stress required to drive shear coupled GB motion may be lower for FCC materials where the Peirels-Nabarro stress is typically less in comparison to BCC systems. Continued investigation of mechanical growth in a wide library of materials is needed to better understand mechanical coarsening across all crystal systems.

3.2 Boundary Character/Structure

The structure of the GB defines its mobility raising the question as to which types of GBs are the most mobile. There is no easy answer. The work by Olmsted et al. [71] suggests that mobility does not correlate well with any of the standard microstructure parameters such as excess volume at the interface, GB energy, misorientation, etc…and experiments by Molodov et al. [24] even show mobility to be sensitive to the inclination of the GB plane. Nevertheless, an attempt is made here to extract a few broad trends with regards to which GBs will be the most mobile.

In his “Theory of grain boundary migration rate” [33] Gleiter considered a GB to be a stepped interface where atoms would detach from a kink on the shrinking grain and re-attach onto a step of the growing grain. For FCC metals, Gleiter’s experiments [82] found these steps to be formed by 111 type planes. Boundaries with high step density and thus a high number of sites for atom detachment would be mobile. Minimum migration rates were therefore predicted for interfaces having orientations parallel to the 111 planes. Gleiter also commented that the migration rate should be dependent on the orientation of the boundary plane, i.e. two boundaries with the same misorientation but a different GB plane orientation can have different mobility values. This last point was more rigorously demonstrated by Janssens et al. [83] using computational methods to show that for FCC metals, mobility is indeed sensitive to the GB plane. A MD simulation study of $\Sigma 3$ boundaries in Al revealed that for a coherent twin, pure

twist about the 111 direction, the mobility was near zero, but if the boundary plane was of the mixed type (rotation axis not normal to boundary plane) then relatively high mobility can be realized. In general, Janssens concludes that "the mobility of mixed-type boundaries is notably higher than the mobility for the pure twist type boundaries."

Taken as a whole it appears that for FCC systems, the mobile boundaries are those of the non-pure twist type whose plane deviates from the 111 type. General trends for hexagonal and BCC structures are unknown as mobility and GBs for these systems have not been widely studied.

3.3 Purity

Purity is well known to have an effect on GB motion as evident by classic work from Cahn [84] detailing how contaminating elements can be adsorbed by a moving interface and dragged along to retard its motion. Studies of GB migration in Pb with the addition of Sn by Aust and Rutter [67] found that increasing the Sn concentration from 0.0004 wt. percent to 0.006 wt. percent can lower the migration rate by a factor of 1,000. This is an interesting observation because while the Sn content was increased by an order of magnitude, the relative content at 0.006 wt. percent is still fairly low. Purity will therefore be especially critical to mechanical growth in nanocrystalline systems, having a high fraction of GB area susceptible to impurity pinning. Gianola et al. [85] demonstrated that mechanical coarsening in sputtered nanocrystalline aluminum films is sensitive to the base pressure during film deposition. Films deposited at pressures around 10^{-5} Torr did not exhibit mechanical growth while films sputtered at 10^{-7} Torr coarsened under tensile loading. The hypothesis from this work was that oxygen and other impurities, more prevalent at higher base pressures, are incorporated into the grain structure pinning the GBs to restrict migration. Using atom probe tomography, quantitative experimental evidence of this premise has now been obtained by Gianola and Tang et al. [86]. Atom probe maps of Al films sputtered at 10^{-5}, 10^{-6}, and 10^{-7} Torr showed significant boundary segregation of oxygen at the highest base pressure of 10^{-5} Torr. Oxygen at 10^{-7} Torr was not detected but segregation was noticeable at 10^{-6} Torr when the oxygen content was only 0.18 atomic percent. MD simulations reinforce this notion that boundaries are highly sensitive to small impurity levels. Elsner [87] simulated a sheared Al bi-crystal having a boundary laced with up to 16 oxygen atoms and it was found that the driving force needed to move the boundary scaled linearly with increasing oxygen content. It is clear that these experimental and computation studies provide strong evidence for mechanical coarsening being sensitive to purity with even a minute impurity content able to pin GBs.

3.4 Loading Conditions

Several mechanical loading schemes have been demonstrated to induce grain coarsening including monotonic events such as quasi static tension [9, 10, 12, 16], compression [13], and indentation [7, 8, 11], severe forms of deformation such as high pressure torsion [78, 80, 88] as well as cyclic loading from fatigue testing [79, 89, 90]. Curiously, for some material systems, only certain loading regimens will result in mechanical coarsening. Nanocrystalline Ni-alloys explored by Padilla and Boyce [89, 90] report mechanical growth occurring on the flanks of cracks formed during fatigue while no growth is detected in the same material tested under static loading. Experiments on nanocrystalline Pt also exhibit this inconsistency. Sharon et al. [12] found growth in nanocrystalline Pt due to tensile loading while Meirom et al. [79] tested nanocrystalline Pt in both tension and fatigue but only observed growth for the cyclic

deformation. The grain structure of the Pt in these works was different as the material from Meirom had columnar grains with strong 111 texture while in the grains in [12] were more random so a direct comparison cannot be made. However, the differences in the behavior of the Pt suggests that depending on the grain structure, only certain loading paths may provide enough driving force to cause coarsening. It could be 111 textured films form boundaries with lower mobility and only migrate once the driving force is elevated from the stress concentration of a fatigue crack.

3.5 Temperature

To elucidate the effect temperature has on the mechanical growth process, the homologous temperature (T_h), a ratio of the test temperature to the melting point of the material is employed. The temperature column of Table 1 lists T_h in brackets for various materials reported to have undergone mechanical growth. Overall, there is no discernible trend to favor the growth process at high or low temperatures. The fact that mechanically driven GB migration readily occurs in Zn at T_h equal to 0.11 and 0.97 suggests some coarsening processes are insensitive to temperature. While the grain growth itself does not appear to be restricted to elevated temperature, this may not be true for the atomic level processes that govern the growth.

To explore this concept in more detail, consider mechanical coarsening examples from two opposite ends of the homologous temperature scale. At a high homologous temperature of 0.86 for Al, GB motion was measured in bi-crystals [91, 92] loaded with an applied shear stress of less than 10^{-1} MPa at temperatures from 500 K to 900 K. The activation energy for such GB migration was determined to be comparable to the activation energy of self and GB diffusion. These experimental findings suggest that the mechanical coarsening occurs via a thermally activated diffusive process.

At the other extreme, mechanical coarsening has been reported in nanocrystalline copper indented at a homologous temperature of 0.06 [8]. Grain growth under conditions of lower thermal energy and higher driving force suggest a coarsening process more mechanical in nature. While experimental limitations prevent complete elimination of temperature, it is possible to conduct purely mechanical simulations. Molecular statics simulations of indented nanocrystalline Al by Sansoz [93] found GB migration activity at 0 K providing support for grain growth being able to occur by a purely mechanical route. Overall, it appears that at high temperatures, the mechanical growth process is more diffusion based but when the temperature is low the process is more mechanical.

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4. PREVALENCE OF MECHANICAL GROWTH IN SMALL GRAINED METALS

Surveying the activity of mechanical growth with respect to grain size, one will find that most room and low temperature coarsening events have been observed in nanocrystalline or ultrafine grained metals. Three aspects unique to small grained systems that may permit this tendency have been identified.

The first aspect is the fact that, in general, fine grained materials can accommodate higher stresses. Coarse grained metals can yield at tens of MPa but decreasing the grain size will increase the yield point following the Hall-Petch [94, 95] trend. For example, the yield point of aluminum has been reported to increase from 50 MPa to 250 MPa when the grain size is reduced from 2 μm to 300 nm [96]. The elevated stresses available to nanocrystalline materials may provide the energy needed to sustain GB migration for prolific coarsening.

Secondly, the processing of small grained materials is quite different from that of bulk systems: the vapor deposition and severe plastic deformation processes often produce grain structures that are not near equilibrium. This instability is evident in several reports of spontaneous room temperature grain growth for nanocrystalline metals [97-99]. In [100], Li notes that GBs in nanocrystalline systems can have "extra" GB dislocations putting them above the lowest-energy state. Li's analysis reveals that the "extra" dislocations make it easier for an applied stress to remove the dislocations that make up the boundary thus deconstructing the interface causing grain growth. The importance of non-equilibrium GBs was also demonstrated in simulations by Tucker at al. [101]. Stressed equilibrium and non-equilibrium GBs in Al and Cu were both found to migrate under loading however the excess free volume from non-equilibrium boundaries "promotes atomic shear shuffling and stress induced atomic rearrangements at lower stresses." Such non-equilibrium boundaries are not expected to be as common in coarse grained metals that are worked and then heat treated with thermodynamics driving the grain structure into a lower energy state. It may be that nanocrystalline processing methods leave the grain structure "unstable" with a higher fraction of boundaries more apt to migrate.

The third aspect is the fact that for nanocrystalline materials, intragranular dislocation based plasticity is suppressed with deformation mediated by GB processes. Alternative mechanisms such as GB sliding [102], creep [103] and partial dislocations emission from the GB [104] have all been proposed but it should also be noted that mechanical coarsening in itself is a deformation mechanism as shear coupled GB migration results in shape changes to grains. Materials will always deform via the mechanism that requires the least amount of energy. For nanocrystalline materials, the energy to deform by dislocation based mechanisms is high so it will be more favorable find an alternate deformation path such as boundary migration.

An additional possibility worth considering is that fine grained materials are not necessarily more prone to mechanical grain growth but that the phenomena is much easier to observe in these materials. Relatively speaking, if GB motion is occurring over short distances (nm scales) then 50-nm of grain boundary motion in a microcrystalline metal would almost certainly go unnoticed whereas 50-nm of boundary migration in a nanocrystalline metal would result in a dramatic change in the grain size.

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5. IMPACT ON MATERIAL RESPONSE

The evolution of a material's grain structure in response to loading can have a noticeable impact on the mechanical behavior. For nanocrystalline metals, mechanical coarsening during deformation can be both a source of failure and a source of extended plasticity.

The Hall-Petch trend is commonly employed to increase strength through grain size reduction. A consequence of this approach is that in most instances the higher strength comes at the expense of ductility. Although possible routes to improve ductility have been proposed [105-107], nanocrystalline metals are still perceived as being "brittle". Mechanical grain growth, as previously stated, is a deformation mechanism because the migrating GB will cause grain shape changes. Therefore, mechanical coarsening provides a path for nanocrystalline materials to accommodate plasticity. Gianola et al. [9] noted that aluminum tested in tension with 40 nm sized grains achieved strengths of ~400 MPa with 5% elongation but did not undergo coarsening. However, from that same study, a somewhat larger grained (90 nm) aluminum achieved lower strengths (149 MPa) but higher elongations (22.4%) when coarsening was active. This observation suggests that the coarsening process enables extended ductility. Analogous reports have been made by Ruan and Schuh [108] who attribute increased ductility for nanocrystalline Al-Mn alloys to deformation induced grain growth. In addition, mechanical grain growth, which is discontinuous, can drive the grain structure to a bi-modal state with both large and small grains. The advantage of having larger grains mixed in with the small is that they will support intragranular dislocation activity and serve as vehicles for work hardening commonly absent from purely nano grained structures. This bi-modal grain size benefit has been demonstrated with thermo-mechanical processed Cu by Wang et al. [109] and further highlighted in [105, 106].

Mechanical grain growth can have the opposite effect as well, initiating material failure instead of delaying it. Cyclic loading of nanocrystalline Ni alloys by Boyce et al. [90] and Pt by Meirom et al. [79] both show mechanical coarsening localized along the flanks of fatigue cracks suggesting that the enlarged grains are more susceptible to crack initiation and advancement. From the experiments, it is unclear if grains coarsen and promote crack nucleation or if the crack forms first and its elevated stress field then drives the grain growth. The former scenario is plausible in light of [110] where mechanical coarsening in nanocrystalline Al films leads to a roughened surface topography with terraces that are potential sites for crack initiation. In [111], Ovid'ko et al. suggests both scenarios are active with the mechanical coarsening not only nucleating a crack but also stunting its advancement. In the developed model, GBs migrate via disclinations which have high local stresses that generate nano-cracks. Once a crack has formed, its growth is slowed as the high stress field at the crack tip is relieved not by advancing the crack but by driving GB motion. It is worth noting that the blunting of a crack tip by GB migration has been observed experimentally [16] however it remains unclear if the mechanical coarsening is the root source of the initial crack formation.

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6. SUMMARY AND CONCLUSIONS

Mechanical grain growth has been discussed with specific focus on the coarsening of nanocrystalline materials at low temperatures. Such grain growth can be reconciled with two new ways of thinking. First, MD simulations suggest the mobility of a GB does not necessarily follow an Arrhenius temperature dependence making it possible to have fast interface motion at and below room temperature. The second is that GB motion is not solely driven be free energy differences between grains but can also occur through stress driven processes. The effects that intrinsic and extrinsic parameters have on mechanical growth are becoming better understood but outstanding ambiguities remain. Glaring issues include the gap between GB mobility studied with simulations and those investigated experimentally. New tools such as precession TEM [112] make the characterization of GBs in nanocrystalline materials possible. Combine this orientation mapping with *in situ* mechanical testing and one can begin to study the mobility of new GB configurations. It is also critical to continue exploring the effects that different crystal structures and different loading conditions have on GB motion. While low temperature mechanical growth was initially reported over 60 years ago [4], the more recent findings of coarsening in nanocrystalline materials continue to reveal the complexity of this phenomenon. Continued investigation, both experimental and computational, is required to obtain a comprehensive understanding.

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