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On the strain-induced stabilization of microstructural features formed along dislocations

M.H. Jhon [a], D.C. Chrzan [b, c], A.M. Glaeser [b, *]

[a] Institute of High Performance Computing, A*STAR, 138632, Singapore
[b] Department of Materials Science and Engineering, University of California, Berkeley, CA 94720, USA
[c] Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

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ABSTRACT

Capillarity-driven mass transport limits the stability of microstructures with a high surface-to-volume ratio. Fiber reinforcements, dendritic structures, and other wire-like morphologies may be susceptible to Rayleigh instabilities and to concurrent or subsequent coarsening. Decreases in the characteristic length scales of microstructures to the nanoscale make such forms of evolution and instability evident at lower values of homologous temperature, consistent with expectations based on size scaling. Herein, we present a simple continuum theory that predicts that sufficiently small second-phase wires exhibiting dislocation character are stable to both Rayleigh instabilities and coarsening. Thus, defects such as hollow-core dislocations will tend to be stabilized while a freestanding nanowire will tend to be unstable. More generally, the effects of surface-energy anisotropy and strain energy on morphological stability are evaluated in a manner that allows their individual and combined effects on stability to be assessed and mapped.

1. Introduction

Modern engineering materials often contain high-aspect-ratio features such as eutectic rod-like microstructures. The utility of these assemblies can be limited at elevated temperatures because of the multifold instability of rod-like structures. Rayleigh instabilities and coarsening are examples of capillarity-driven modes of microstructural instability; both cause morphological changes with potentially deleterious effects on material properties. They reduce the excess interfacial energy per unit volume, and decrease the interface-to-volume ratio in isotropic systems.

The Rayleigh instability, sometimes referred to as pearling or fragmentation, refers to the susceptibility of an individual rod to the growth of periodic axial perturbations having a wavelength λ exceeding a critical minimum value, as shown in Fig. 1. This process will eventually lead to rod breakup into an array of equiaxed structures [1]. Coarsening, or Ostwald ripening, refers to a process in which a dispersion of particles or precipitates progressively increases its mean size through diffusional interactions. This process can be interpreted as the growth of larger particles at the expense of the smaller ones.

These two modes of microstructural evolution become more pronounced for smaller features. Based on scaling-law arguments for self-similar morphological changes through surface and interface diffusion [2], the time required for Rayleigh breakup is proportional to R_0^4, where R_0 is the unperturbed rod radius. Thus, a tenfold decrease in R_0 is expected to reduce the breakup time by a factor of 10^4. Likewise, the coarsening rate increases as the mean precipitate or particle size decreases. Again assuming self-similarity, the mean rod radius increases with time t at fixed temperature, and is proportional to $t^{1/3}$ or $t^{1/4}$, depending upon the dominant growth mechanism [3]. In other words, the rate of change is highest at short times when the average size is smallest.

The predicted time and size dependencies for coarsening and Rayleigh breakup indicate that stabilization of the fine-scale structures of current interest will pose tremendous challenges that will become increasingly severe as dimensional scales are further reduced. This has already been observed in a variety of nm-scale systems. For example, studies of the morphological evolution of Au nanowires with $R_0 = 12.5 - 66$ nm show that breakup can occur in <30 min at 300 °C for the finest-size fibers [4]. As R_0 is decreased, breakup occurs in less time at fixed temperature, and at lower temperature for fixed anneal time. Similar trends are suggested by studies of Cu nanowires ranging from 30 nm to 120 nm in

* Corresponding author.
E-mail address: aglaeser@sapphire.berkeley.edu (A.M. Glaeser).

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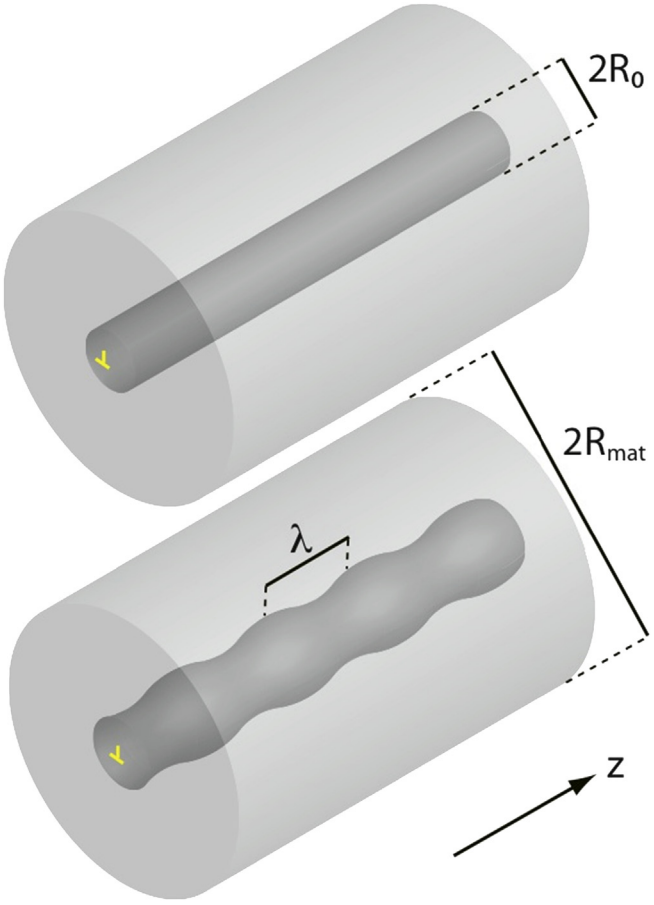

Fig. 1. Schematic illustration of a rod-like particle grown on a dislocation line and undergoing a Rayleigh instability with a characteristic wavelength λ. The top panel depicts the rod prior to the development of a discernible perturbation, while the lower panel shows the rod after the perturbation is well developed. The light grey region represents the matrix phase and the dark grey the precipitate phase. The dislocation line extends parallel to the axis of the cylinder.

diameter; fragmentation of 40-nm diameter wires occurs in as little as 20 min at 400 °C [5]. For Ag, "10-nm in diameter" nanobelts undergo fragmentation at room temperature. Kolb et al. [6] have shown that Si-core–SiO_2-shell wires with diameters >100 nm develop periodic variations in the inner (Si) and outer (SiO_2) radii, and breakup of the Si core can occur in the 900–1000 °C range in times as short as 2 h. These reported instances of fiber instability or nanowire "decomposition" may reflect Rayleigh instabilities, and additional examples are likely to emerge.

Prior work has shown that the presence of surface-energy anisotropy can delay breakup and stabilize fibers and internal rod-like voids [7]. The present work considers the ability of strain energy to stabilize nanowires and nanowire arrays, and the combined effects of strain energy and surface-energy anisotropy are explored. Specifically, we examine the consequences of the strain field of a dislocation on both the coarsening and Rayleigh instability of single-crystal nanowires grown along dislocations. The analysis is also relevant to the rod-like voids known as hollow-core dislocations, as found in GaN [8] and SiC [9]. We show that strain energy alone can fully suppress both coarsening and the Rayleigh instability when R_0 is sufficiently small, and that elastic strain energy and surface or interfacial-energy anisotropy working in tandem can delay breakup significantly at larger R_0. This suggests strategies for fabricating nanowire arrays suited for use at elevated temperatures where diffusion is active.

2. Background

Various strategies have been developed to stabilize microstructures with a high interface-area-to-volume ratio, typically by modifying the driving force for microstructural change. For example, the initial particle-size distribution of a powder can be narrowed, generating very fine grain size by reducing the driving force for coarsening [10]. In systems such as age-hardenable Ni alloys, the precipitate/matrix interfacial energy is low, reducing the interfacial-energy component of the driving force for coarsening [11]. Similarly, decreasing the solubility of the dispersed phase in the surrounding matrix or the diffusivity of the precipitate constituent decreases the solubility-diffusivity product and thus the chemical driving force for microstructural change [12].

A particularly important strategy for stabilizing high-aspect-ratio structures is to carefully choose the system crystallography to exploit surface-energy anisotropy. Cahn [13] first formulated this effect in the context of the Rayleigh breakup of a rod with anisotropic surface energy. The analysis assumes that the surface energy is radially isotropic in sections normal to the rod axis, resulting in a circular cross section. Anisotropy arises when axial variations in the radius incline the surface by an angle $\phi = \partial R/\partial z$ to the rod axis. Surface-energy anisotropy significantly alters rod breakup. In systems with isotropic surface energy, the rod is unstable to fluctuations with $\lambda > \lambda_{\min}^{iso} = 2\pi R_0$. However, when the orientation of the unperturbed surface lies in a local surface-energy minimum, the minimum wavelength for instability, $\lambda_{\min}$ is increased relative to $\lambda_{\min}^{iso}$. When the unperturbed surface lies in a cusp orientation, the rod is stabilized against all infinitesimal perturbations. Stölken and Glaeser [14] assessed the impact of such surface-energy-anisotropy-induced stabilization on surface- and interface diffusion-controlled evolution, and showed that the kinetically dominant wavelength, $\lambda_{\max}$, is also shifted, but the ratio of $\lambda_{\max}/\lambda_{\min}$ remains $\sqrt{2}$, unchanged from that of isotropic systems. Surface-energy anisotropy strongly affects the kinetics of breakup: each factor of n increase in $\lambda_{\min}$ is expected to increase the breakup time by a factor of n^2. More recent contributions to this topic have addressed more complex forms of the surface-energy anisotropy, including transverse anisotropy [15].

Strain energy can likewise modify the driving force for capillarity-driven processes. For coarsening processes, strain interactions have been implicated as the basis for the development of aligned, or periodic arrays of discrete precipitates in bulk alloys, and conditions have been formulated that would lead to inverse coarsening, a narrowing of the size distribution and the development of stable monosized arrays of particles [16]. Sridhar et al. [17] found that misfit strains may alter the wavelengths for which a rod is susceptible to the Rayleigh instability. However, misfit strains only reduce the driving force for Rayleigh breakup; they cannot completely stabilize a wire. On the other hand, the strain energy of a dislocation has been predicted to stabilize high-aspect-ratio structures. Frank [18] proposed that if the surface energy is sufficiently low, the cores of dislocations could open to form a hollow-core dislocation or "micropipe" as a means of reducing the elastic-strain energy of a system. Such hollow-core structures have been observed experimentally in a number of systems, including GaN [19], SiC [20], and AlN [21]. These structures are unusual because they are voids that exhibit the strain field associated with dislocations. Their shape is determined by balancing the strain-energy reduction of an open core with the energy penalty for creating new surfaces. Their equilibrium radius was estimated to be $R_f = A/2\pi\gamma_{sv}$, where A is $Gb^2/4\pi(1-\nu)$ for an edge dislocation and $Gb^2/4\pi$ for a screw dislocation, G the shear modulus, b the length of the Burgers vector, ν Poisson's ratio, and γ_{sv} is the solid-vapor interfacial energy. However, the theory of Frank [18] was not able