Scripta Materialia 113 (2016) 167–170

Contents lists available at ScienceDirect

Scripta Materialia

journal homepage: www.elsevier.com/locate/scriptamat

Detachment of nanowires driven by capillarity

Fei Wang *, Britta Nestler

[a] Institute of Materials and Processes, Karlsruhe University of Applied Sciences, Moltkestrasse 30, 76133 Karlsruhe, Germany
[b] Institute of Applied Materials–Computational Materials Science, Karlsruhe Institute of Technology (KIT), Haid-und-Neu Strasse 7, 76131 Karlsruhe, Germany

ARTICLE INFO

Article history:
Received 10 October 2015
Accepted 1 November 2015
Available online 19 November 2015

Keywords:
Nanowire
Detachment
Capillarity
Plateau–Rayleigh instability
Surface diffusion

ABSTRACT

The spontaneous breakup of nanowires into nanospheres is of crucial significance preventing it from applications. In the present work, we propose a generalized stability criterion for nanowires, in contrast to the convectional Rayleigh stability theory that has been widely employed to understand the breakup-mechanism of nanowires. We demonstrate that the minimum instability wavelength is $\lambda_{critical} = 2\pi\sqrt{R_0^2 - a^2}$ in contradiction to the convectional Rayleigh condition $\lambda_{critical} = 2\pi R_0$, where R_0 and a are the radius of the nanowire and the amplitude of the perturbation, respectively. The modified theory is confirmed by the dynamic phase-field simulations of different nanowire shapes.

Metallic and semiconductor nanowires play essential roles in nanoelectronics, optoelectronics, sensorics, and numerous other fields [1,2,3,4,5]. Thermal annealing is often applied on nanowires as a post-fabrication treatment to achieve desired physical properties [6,7]. During the thermal annealing process or even at room temperature, nanowires may fragment into a chain of nanospheres [8,9,10,11], which prevents it from applications. Also, nanospheres are purposely produced from nanowires in microelectronic industry where the grain size affects the electrical resistance and is hence of significant relevance [12].

The evolution of nanowires into nanospheres has been extensively explained by the Rayleigh instability theory [13,14,15,16,17,10,18,19]. If we consider a nanowire with radius R_0 perturbed by a sinusoidal function in the radial direction $R = R_0 + a\sin(2\pi z/\lambda)$, the minimum wavelength to cause the detachment is the circumference of the nanowire $\lambda_{critical} = 2\pi R_0$ according to Rayleigh's theory [20].

In the present work, we show that for $\lambda < 2\pi R_0$, the detachment of nanowire is able to take place depending on the perturbation amplitude, which is in conflict with the classical Rayleigh theory. The minimum perturbation wavelength $\lambda_{critical}$ as a function of the perturbation amplitude a for $\lambda < 2\pi R_0$ has been analytically derived. Moreover, we demonstrate the modified theory by numerical experiments based on the phase-field method.

As shown in Fig. 1(a), the atoms of a planar interface of nanowire-environment are regularly ordered along the interface and therefore, the chemical potentials for atoms and vacancies are both uniformly distributed, establishing the thermodynamic equilibrium between the nanowire and environment. While the interface is stirred by a sinusoidal function, the potential energies along the interface of the nanowire are inhomogeneous because of non-uniformly distributed mean curvature. With contributions from the mean curvature, the diffusion potential energy is expressed as [21]

$$\Phi = \mu_A^0 + \gamma\Omega\kappa, \tag{1}$$

where μ_A^0 is the chemical potential of a planar interface as a reference state illustrated in Fig. 1(a), γ is the isotropic interfacial energy, Ω is the atomic volume, and κ is the signed mean curvature. For instance, in two dimensions, the diffusion potentials at $\lambda/4$ and $3\lambda/4$ are $\Phi_{\lambda/4} = \mu_A^0 + \gamma\Omega|\kappa|$ and $\Phi_{3\lambda/4} = \mu_A^0 - \gamma\Omega|\kappa|$, respectively (see Fig. 1(b)). The gradient of the diffusion potential energy $-\nabla\Phi \propto 2\gamma\Omega\nabla\kappa$ in turn induces a surface flux from $\lambda/4$ to $3\lambda/4$, as schematically sketched in Fig. 1(c), smoothing the nanowire.

We highly emphasize that for a three-dimensional surface $x = f(y,z)$, κ in Eq. (1) is the mean curvature rather than individual principal curvatures. For a nanowire (radius R_0, length $n\lambda$, n is an integer) perturbed by a sinusoidal function in the radial direction $R_0 + a\sin(2\pi z/n\lambda)$, the mean curvature of the interface is defined as $\kappa \equiv \frac{1}{2}\nabla\cdot\mathbf{n}$, where $\mathbf{n}$ is the normal vector expressed as $\mathbf{n} = (-1, \partial_y f(y,z), \partial_z f(y,z))$, with $f(y,z) = \sqrt{[R_0 + a\sin(2\pi z/\lambda)]^2 - y^2}$.

* Corresponding author at: Institute of Materials and Processes, Karlsruhe University of Applied Sciences, Moltkestrasse 30, 76133 Karlsruhe, Germany.
E-mail addresses: fei.wang@hs-karlsruhe.de (F. Wang), britta.nestler@kit.edu (B. Nestler).

http://dx.doi.org/10.1016/j.scriptamat.2015.11.002
1359-6462/

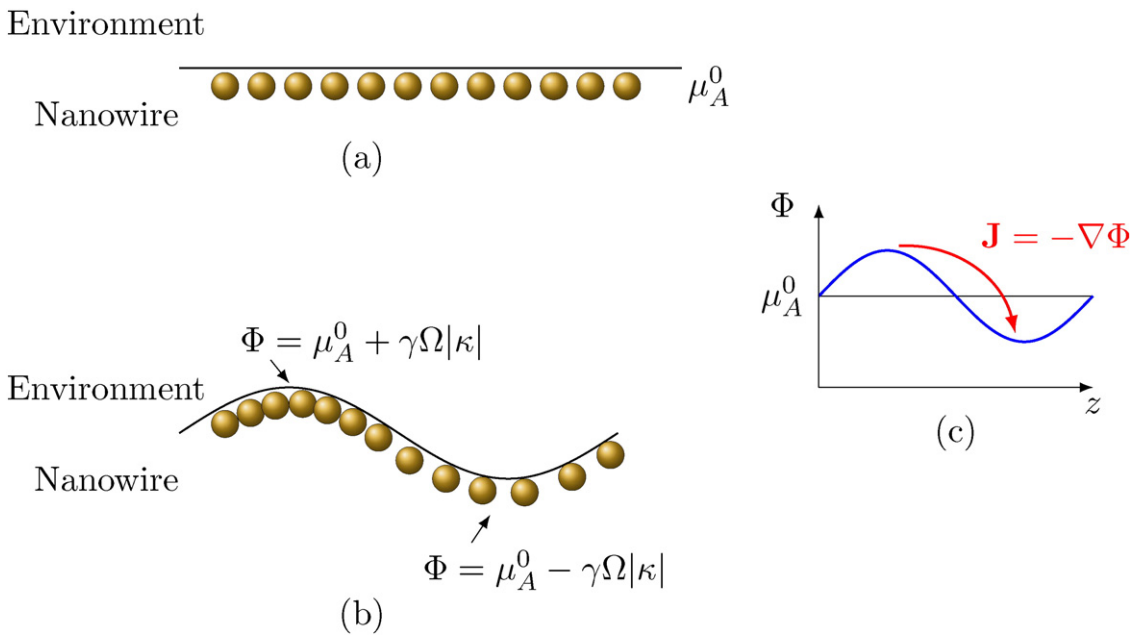

Fig. 1. Schematic illustration for chemical potential distribution affected by curvature: (a) The chemical potential is uniform distributed for a planar interface. (b) The chemical potential along the interface of the nanowire is inhomogeneous because of perturbations. (c) A surface flux is induced by the gradient of diffusion potential Φ.

Exploiting the axi-symmetrical geometrics, the mean curvature only depends on the longitudinal variable z

$$\kappa(z) = \frac{1}{2}\left\{ \underbrace{\frac{a(2\pi/\lambda)^2 \sin(2\pi z/\lambda)}{\left[1+(2a\pi/\lambda)^2\cos^2(2\pi z/\lambda)\right]^{3/2}}}_{\text{longitudinal curvature}} + \underbrace{\frac{1/[R_0 + a\sin(2\pi z/\lambda)]}{\left[1+(2a\pi/\lambda)^2\cos^2(2\pi z/\lambda)\right]^{1/2}}}_{\text{radial curvature}} \right\}, \tag{2}$$

where the first term is the principal curvature contribution from the longitudinal direction and the second term is the dedication from the radial direction. For $z=\lambda/4$ and $z=3\lambda/4$, we obtain $\kappa_{\lambda/4} = \frac{1}{2}[a(2\pi/\lambda)^2 + 1/(R_0+a)]$ and $\kappa_{3\lambda/4} = \frac{1}{2}[-a(2\pi/\lambda)^2 + 1/(R_0-a)]$. It is evident that $a(2\pi/\lambda)^2$ and $-a(2\pi/\lambda)^2$ are the curvatures as the ones in two dimensions and $1/(R_0+a)$ and $1/(R_0-a)$ are the curvature contributions from the third dimension.

The distribution of the mean curvature in the longitudinal direction z is illustrated in Fig. 2(a) for different perturbation amplitudes. The corresponding geometric setting is $\lambda/d_0=160$ and $R_0/d_0=30$, where d_0 is the capillary length. For small amplitudes, e.g., $a/d_0=3$, the mean curvature decreases monotonically from λ/4 to 3λ/4, as shown by the red solid line. In this case, the potential energy Φ at λ/4 is greater than the one at 3λ/4, since $\kappa_{\lambda/4} > \kappa_{3\lambda/4}$. The difference in the diffusion potential Φ consequently induces a surface flux $\mathbf{J}_1$ from λ/4 to 3λ/4, as sketched in Fig. 2(b). The subsequent effect is that the interface contracts towards the center of the nanowire at λ/4 and bulges out at 3λ/4. The nanowire evolves till the interface becomes flat and the respective diffusion potential Φ is uniformly distributed along the interface. This monotonic decrease of the mean curvature from λ/4 to 3λ/4 is comparable to the situation in two dimensions.

With an increase of the amplitude, extrema of the mean curvature occur between λ/4 and 3λ/4, as illustrated by the green, blue and magenta lines in Fig. 2(a). The locations of the curvature extrema for $a/d_0=8,13$ and 18 are denoted by z_1, z_2 and z_3, respectively. The corresponding potential energies Φ at λ/4 and 3λ/4 are both greater than the ones at z_i, $i=1,2,3$. Hence, two surface fluxes take place between λ/4 and z_i and between 3λ/4 and z_i, as schematically depicted by $\mathbf{J}_1$ and $\mathbf{J}_2$,

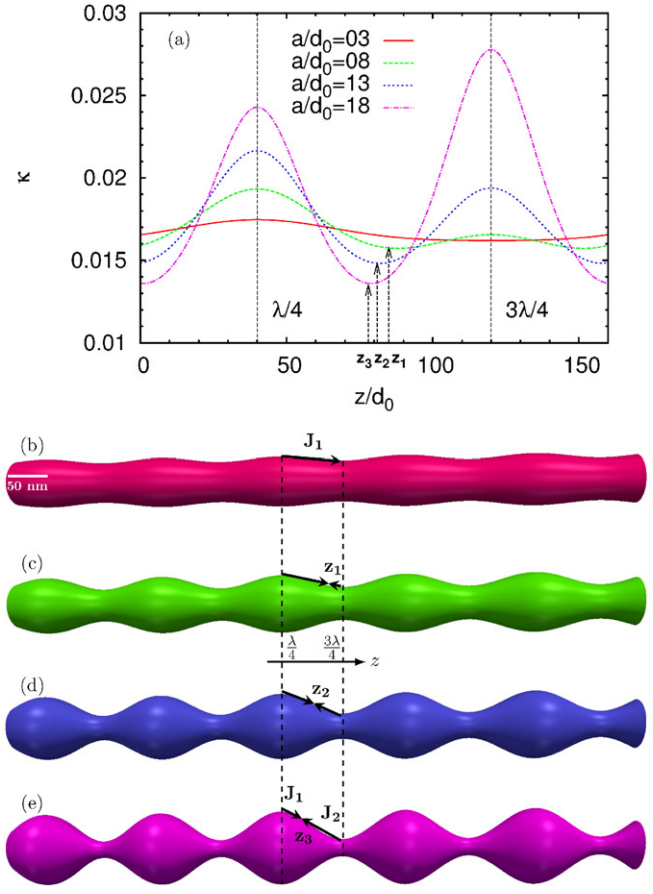

Fig. 2. Effect of curvature distribution on the surface flux for stirred nanowires: (a) Mean curvature as a function of the spatial variable in the longitudinal direction for different perturbation amplitudes. (b), (c), (d), and (e) schematic drawings of the directions of the surface fluxes for perturbations with amplitudes $a/d_0=3,8,13,18$, which correspond to the red, green, blue and magenta lines in (a), respectively.