Length-dependent mechanical properties of gold nanowires

Jing Han,¹ Liang Fang,^{1,2,a)} Jiapeng Sun,^{2,b)} Ying Han,² and Kun Sun²

¹*School of Mechanical and Electrical Engineering, China University of Mining and Technology, Xuzhou, 221116 Jiangsu Province, People's Republic of China*

²*State Key Laboratory for Mechanical Behavior of Materials, Xi'an Jiaotong University, Xi'an, 710049 Shaanxi Province, People's Republic of China*

(Received 11 August 2012; accepted 6 November 2012; published online 6 December 2012)

The well-known “size effect” is not only related to the diameter but also to the length of the small volume materials. It is unfortunate that the length effect on the mechanical behavior of nanowires is rarely explored in contrast to the intensive studies of the diameter effect. The present paper pays attention to the length-dependent mechanical properties of $\langle 111 \rangle$ -oriented single crystal gold nanowires employing the large-scale molecular dynamics simulation. It is discovered that the ultrashort Au nanowires exhibit a new deformation and failure regime—high elongation and high strength. The constrained dislocation nucleation and transient dislocation slipping are observed as the dominant mechanism for such unique combination of high strength and high elongation. A mechanical model based on image force theory is developed to provide an insight to dislocation nucleation and capture the yield strength and nucleation site of first partial dislocation indicated by simulation results. Increasing the length of the nanowires, the ductile-to-brittle transition is confirmed. And the new explanation is suggested in the predict model of this transition. Inspired by the superior properties, a new approach to strengthen and toughen nanowires—hard/soft/hard sandwich structured nanowires is suggested. A preliminary evidence from the molecular dynamics simulation corroborates the present opinion. © 2012 American Institute of Physics. [<http://dx.doi.org/10.1063/1.4768284>]

I. INTRODUCTION

Motivated by the potential application successively in shrinking modern electronic devices, the plastic deformation of small volume metal crystals on micro- and nanoscale, such as whiskers, nanowires, and nanopillars, has been attracting considerable attention recently. In particular, Au nanowires have been exerted a great deal of effect as a promising candidate for future interconnections and an active component^{1,2} because of its excellent electrical and mechanical properties and the desired chemical inertness.

When the diameters of the samples reduce to the nanoscale, namely nanowires, the materials reveal unique mechanical behaviors in comparison of the bulk counterparts. For example, single-crystalline face-centered cubic (fcc) metal nanowires exhibit “smaller is stronger” trend,^{3–5} and its plastic deformation mechanism shifts from dislocation multiplication via the operation of Frank-Read sources⁶ for bulk material to dislocation nucleation originated either single-arm sources⁷ or surface sources⁸ as its diameter decreases to nanoscale.⁹ Almost all the atomistic simulations have predicted that stress-strain curves of the single crystal fcc metal nanowires exhibit high strength (in the gigapascal range vs megapascal for their bulk counterpart), lack of hardening, and ductile failure.^{10–14} Some experiments verify these viewpoints,^{15–17} but other experiments find single crystal fcc metal nanowires can fail through either brittle fracture without noticeable ductile necking or localized shear failure without extensive plasticity.^{18,19} The distinctions between the experiments and atomistic simulation imply something

haunts us. Wu²⁰ regards the length of nanowires as the culprit. They show a ductile-to-brittle with increasing Cu nanowires length, which spans the experiments and the atomic simulation results firstly.

In the present work, the length-dependent mechanical properties of the single crystal gold nanowires are investigated employing the large-scale molecular dynamics (MD) simulation. We shed specific light on the deformation and failure of the ultrashort Au nanowires (<24.00 nm). The results indicate that the ultrashort Au nanowires exhibit exciting combination of high elongation and high strength under tensile deformation. To explain this observation, we develop a theoretical model to provide an insight to dislocation nucleation and capture the yield strength and nucleation site of first partial dislocation. Furthermore, more nanowires with a large range of lengths are also investigated in order to entirely map the length-dependent deformation behavior of the nanowires. Finally, a new approach to strengthening and toughening materials—hard/soft/hard sandwich structured nanowires is suggested inspired by the superior properties of ultrashort nanowires. The sandwich structured nanowires also provide a possible experimental method to verify the unique properties of ultrashort nanowires discovered by the molecular dynamics simulation. The present work suggests an understanding of engineering principles in designing the nanoscale devices.

II. METHODOLOGY

Large-scale molecular dynamics simulations are performed with an embedded atom-method potential²¹ to determine the tensile deformation of $\langle 111 \rangle$ -oriented Au nanowires with closed circle cross section. In order to consider the end

^{a)}E-mail: fangl@xjtu.edu.cn.

^{b)}E-mail: sun.jiap@gmail.com.

FIG. 1. Atomic model of single crystal gold nanowires.

effect of the nanowires, the free boundary condition other than periodic condition is adopted along the axial direction of the nanowires. In other words, the finite length nanowires other than infinite length nanowires are studied in the present paper. The present model consists of an internal deformation layer, a fixed layer, and a loading layer, which is used to load, as shown in Fig. 1. The fixed layer and loading layer are set as rigid with same thickness of ~ 0.82 nm. The initial diameter of all the nanowires is chosen to be ~ 6.66 nm, and the initial length (the length of the internal deformation layer) is chosen from a range of 3.53–1060.02 nm. To suppress the oscillation of the axial stress led by the low frequency but long-lived oscillations associated with the free boundary,²² the stochastic thermostat-Langevin dynamics²³ is used for the 300 K thermal equilibrium at the beginning of the simulation. Later, the uniaxial tension is simulated by displacing the atoms in loading layers at a constant strain rate of $5e7$, which is low enough to retain the dislocation plasticity rather than amorphous plasticity,²⁴ but the atoms in fixed layer are frozen. The nanowires maintain constant temperature of 300 K by the Nose-Hoover thermostat^{25,26} on the stretching process.

III. RESULTS

A. Length-dependent mechanical behavior and atomic mechanism

Figs. 2(a)–2(d) show the engineering stress-strain curves of four Au $\langle 111 \rangle$ nanowires at length $L = 3.53, 7.07, 106.00$, and 1060.02 nm. The unique combination of high-strength of ~ 4.98 GPa and high-elongation of $\sim 275.18\%$ are impressive for the 3.53 nm nanowire. The 7.07 nm nanowire also exhibits excellent combination of high-strength (~ 4.19 GPa) and high-elongation ($\sim 174.03\%$). Fig. 2(e) illustrates the elongation, yield strength, and elastic modulus related to the nanowires length. It indicates the yield strength and elongation increases abruptly when the length of the nanowire is reduced less than ~ 21.2 nm, but the variation is gentle for the long nanowires. The sudden changes of the yield strength and the elongation imply the transition of deformation mechanism. While the elastic moduli are almost constant for all nanowires. In addition, some other characteristics of stress-strain as reported in reference also appear in Fig. 2, such as a sharp drop in stress following the approximate linear elastic and a series of the serrations indicating the discrete dislocation events, etc.

In order to probe the originations of the high strength and high elongation, we investigate the atomic process that occurs during deformation until the final fracture, as illustrated in Fig. 3. It shows that, for all the nanowires, the first plasticity event is facilitated by the nucleation of the partial dislocation associated with the formation of a stacking fault. After the first dislocation nucleation event, all the nanowires exhibit multiple bursts of dislocation activities at different locations in different slip systems, and then produce many shear facets over a large region of the wires. These multiple bursts of dislocation dissipate the accumulated strain energy that results in the multiple serrations of the stress-strain

FIG. 2. Panels a–d illustrate the engineering stress-strain curves for the four nanowires at different initial lengths. The insert to panel a shows enlarged stress-strain curves in small deformation. Panel e shows the elongation, yield strength, and elastic modulus related to nanowires length.

FIG. 3. Snapshot of the plastic deformation of 3.53 nm (panels a1-a3), 106.00 nm (panels b1-b3), and 1060.02 nm (panels c1-c4) nanowires, corresponding to labeled points in Figs. 1(a), 1(c), and 1(d), respectively. Atoms are shown only if their common atomic neighborhood^{27,28} differ from that of the perfect fcc crystal. The atoms of hcp crystal are shown in blue. The atoms of other than fcc, bcc, hcp, and icosahedral crystal are shown in red. Panels a4 and b4 illustrate the occurring of necking. Panels a5, b5, and c5 show the fracture morphology.

curves, as shown in Fig. 1. The maxima of the serrations corresponds to the stress required to activate the dislocation slip processes, and the minima indicates the termination of the dislocation slip processes. So each serration represents the dissipation and subsequent accumulation of the strain energy.

Although many common deformation features are exposed for all the nanowires as the aforementioned, the 3.53 nm nanowire reveals some substantially different atomic level processes during deformation. The 3.53 nm nanowire undergoes first stress dropping resulted by the free surface-induced heterogeneous nucleation of partial dislocation as shown in Fig. 3(a1), but the partial dislocation cannot slip freely. Thus, more dislocations located at all six probable slip systems will nucleate and slip transiently, and then leave behind the intrinsic stacking fault for dissipating the accumulated strain energy. Subsequently, the stacking faults interaction gives rise to a network of stacking faults in the nanowires, and the drop of stress to a minimum, as shown in Fig. 3(a2). Increasing the strain, the trailing partial dislocations will diminish even vanish the stacking fault, as shown in Fig. 3(a3), which leads to the increasing of stress until the nucleation of new partial dislocations. Therefore, such dislocation nucleation, motion, and interaction processes repeating endlessly cause the serrations of the stress-strain curves. The 7.07 nm nanowires have the same dislocation mechanism as the 3.53 nm nanowires. The only discrepancy is that not all the six probable slip systems are active due to the weak obstacle resulted by the slightly large length.

With extensive stretching, faceted nanowires with immobile stacking fault confine the subsequent nucleation and motion of additional dislocations. As a result, necking occurs and the stress drops abruptly to dissipate the accumulated energy. Before the necking, the nanowires undergo stable deformation (the dislocation process is described as above) and the stresses reduce slowly, as shown in Fig. 1 (at

the point a4 and b4, the necking occurs). The 3.53 nm and 7.07 nm nanowires remain uniform diameters during deformation because of a succession of transient slip motion of a great number of dislocations in multiple distinct slip system. Even if the necking occurs, the 3.53 nm and 7.07 nm nanowires still need a longer period of dislocation plasticity before they fail. But any other samples fracture fast once the necking happens after the short stable deformation. So it can be concluded that the high elongation is attributed to the constrained dislocation motion characterized by the transient slipping of a large number of dislocations in multiple distinct slip system, and is dominated by whether the deformation can spread the entail length.

B. Theoretical model for the high-strength of the ultrashort nanowires

The super compression strength of short nanobutons also has been reported by Rinaldi²⁹ on the experiments. The authors attribute the high-strength to the extra quota of load leaded by the base and the multiaxial stress distributes around the substrate. In the present paper, the similar high-strength is shown for the ultrashort single crystal Au nanowires. The finite element (FE) model of 3.53 nm nanowire (Young's modulus $E = 130.0$ GPa, Poisson's ration $\nu = 0.3$) illustrates that there are a multiaxial stress and large stress gradient, as shown in Fig. 4. The maximum stress presents in the corner of the tip. Thus, the FE model predicts the first partial dislocation nucleation site locates at the tip of the nanowires. This prediction departs from the molecular dynamics simulation results. Thus we could infer that the multiaxial stress is not the dominant mechanism. We will reveal that the constraint from the fixed atoms to the nucleation of first partial dislocation is primarily responsible for the high-strength. The constraint can be expressed by a virtual force, i.e., image force τ_f . To evaluate the image force, a "two-phase" model can be applied if the matrix and the fixed atoms are treated as materials of different shear moduli. Considering a straight pure screw dislocation of infinite length, τ_f originating from the fixed atoms can be evaluated by

$$\tau_f = \frac{b\mu_1}{4\pi r} \left(\frac{2\mu_2}{\mu_1 + \mu_2} - 1 \right), \quad (1)$$

where b is the Burgers vector, μ_1 and μ_2 the shear moduli of matrix and fixed atoms, respectively, r the distance from the

FIG. 4. Radial stress (panel a) and axial stress (panel b) component for the axisymmetric model of a nanowire ($D = 6.66$ nm, $L = 6.66$ nm) stretched by a rigid displacement. The stress field corresponds to an applied strain of about 0.016.

interface of the two materials. Considering that μ_2 is infinite, the explicit form of τ_f when $\mu_2 \rightarrow +\infty$ is

$$\tau_f = \frac{b\mu_1}{4\pi r}. \quad (2)$$

The dislocation nucleation locates at $h*L$ away from the below fixed atoms. The distance r_u between the up fixed atoms and dislocation, and r_b between the below atoms and dislocation can be approximated as follows:

$$\begin{aligned} r_u &\approx \frac{L(1-h)}{\sin \theta}, \\ r_b &\approx \frac{h}{\sin \theta}L, \quad 0 < h \leq 0.5, \end{aligned} \quad (3)$$

with θ being the angle between the fixed layers and $\{111\}$ slip plane, and L the length of the nanowires. The image force from the up and below fixed atoms can be inferred by combining Eqs. (2) and (3) as follows:

$$\tau'_f = \lambda \frac{b\mu_1 \sin \theta}{4\pi L}, \quad \lambda = \frac{1}{h(1-h)}. \quad (4)$$

The prefactor λ represents the dislocation nucleation site. The critical resolved shear stress (CRSS, τ_{CRSS}) for the dislocation nucleation can be written as follows:

$$\tau_{CRSS} = \tau_0 + \lambda \frac{b\mu_1 \sin \theta}{4\pi L}. \quad (5)$$

Here, the first term τ_0 is the resolved shear stress for dislocation nucleation losing the image force. It is notable that, Eq. (5) illustrates the first dislocation nucleation tends to the center of the nanowires because of the image force obtained minimum value with $h = 0.5$. The molecular dynamics simulations result that the first partial dislocation nucleates locating at $h \approx 0.40$ for the 3.53 nm nanowire, which is close to the theory predication but deviates from the FE results.

And then, we will evaluate quantitatively the image force. In the present paper, taking $\mu_1 = 23.667$ GPa, $b = 0.16657$ nm, $\sin \theta = 2\sqrt{2}/3$, and $h = 0.5$, the minimum image force can be calculated as

$$\tau'_{fmax} = 11.83/L. \quad (6)$$

Thus, the image force (~ 0.050 GPa) loses the domination to CRSS when the length is larger than ~ 24.03 nm. So the length ~ 24.03 nm can be regarded as the critical length L_{min} to assess the effect of the image force. The image force will affect the CRSS significantly while $L < L_{min}$, but will tend to vanish with large length. Assuming the invariant dislocation nucleation sites, the CRSS will be inversely proportion to the length of nanowires. The CRSS from the molecular dynamics which is calculated by multiplying the yield stress by the Schmid factor 0.314 can be fitted using Eq. (5) to evaluate the τ_0 and the λ . The result is plotted in Fig. 5. The fitted λ and τ_0 is 6.60 and 1.03 GPa, respectively. In summary, we conclude that the high-strength is resulted by the enhanced CRSS for dislocation nucleation by the fixed layer atoms.

FIG. 5. The predict by the mechanical model vs. molecular dynamics simulation.

C. The ductile-to-brittle transformation increasing the length of the nanowires

In this section, we discuss the deformation behavior of long nanowires. The critical length L_c that the brittle failure occurs equals $d \cot \alpha / \varepsilon_y$ (d is the diameter, ε_y is the yield strain).²⁰ Although this criterion agreed well with the simulation results in Wu's studies, the selection of the parameter α is not stated clearly. If the plastic deformation is just carried by leading partial dislocation, the parameter α should be the angle between the slip directions of partial dislocation and the stretching axis ($\cot \alpha = 2\sqrt{2}$). Considered here ($d = 6.66$ nm, $\varepsilon_y \approx 0.024$), L_c equals 784.89 nm. While the plastic deformation is mediated by leading partial dislocation and subsequent trailing partial dislocation which is equivalent to a perfect dislocation, the $\cot \alpha$ equals $\sqrt{2}$, and L_c equals 392.44 nm. In other words, once trailing partial dislocation is emitted, the critical length L_c should be in the range of 392.44–784.89 nm. Our molecular dynamics show that the critical length is 706.68 nm, which confirms the predict results. It also indicates that the plastic deformation of nanowires is dominantly mediated by the leading partial dislocation and few trailing partial dislocations are emitted. If this critical condition is met, the nanowires exhibit extreme shear localization and fail abruptly, as shown in Fig. 2(e). And there are no longer the serrate characteristics on the stress-strain curves. The first dislocation even is facilitated by nucleation of multiply partials located at distinct slip system, other than only one nucleation of partial for the short nanowires, as shown in Fig. 3(c1). Subsequently, multiple bursts of dislocation activate and slip, leaving complicated stacking faults networks in the nanowires. Eventually, shear deformation along the stacking faults region develops rapidly at localized region, causing the nanowire to rupture without noticeable necking.

IV. DISCUSSION

We have attributed the unique combination of high-strength and high-elongation of the ultrashort nanowires to the constrained partial dislocation nucleations and motions induced by the fixed ends. One argument about the superior property is the realization in the experiments because it is unrealistic that the rigid fixed ends adopted in the molecular dynamics simulation. In fact, the rigid fixed ends in the

simulation can be regarded as an assumed material which possesses the same crystal structure and infinite shear moduli. In our predictive model, the enhanced strength is derived from the essentially large shear moduli of the fixed ends, but not related to the crystal structure of the fixed ends. The high elongation is only related to the dislocation blocked by the interface. Hence, the materials with large shear moduli and favorable interface with the nanowires can be used to achieve the high strength and high elongation of the ultrashort nanowires instead of fixed ends. In view of the above, we can suggest a new approach, hard/soft/hard sandwich structured nanowires, to strengthen and toughen the nanowires. For example, the studied ultrashort soft nanowire is joined with hard nanowires at both ends, as shown in Fig. 6. In this sandwich structure, the hard ends can still constrain the partial dislocation nucleations and motions and then achieve the high strength and high elongation of the ultrashort soft metallic nanowire, which has similar results with our previous simulation model. It is worth notable that the sandwich structured nanowires (as shown in Fig. 6) can be already fabricated by the existing technologies. For instance, the hard nanowires can be joined to the soft nanowires utilizing cold welding technology^{30,31} or even directly gluing. Otherwise, the sandwich structure nanowires can be obtained by using Focused Ion Beam (FIB)³² machining technology or reactive-iron etching³³ to carve the multilayer nanofilms, which can be created by the techniques already established, such as sequential sputtering,³⁴ electrodeposition,³⁵ or electron-beam lithography. Nevertheless, the selection of a suitable pair of hard and soft metals is difficult because the interface of the two metals should be strength enough to block the dislocation and prevent premature fracture on the interface. We can find a cue from few references. Y. Lu *et al.*³⁶ have reported an ultrahigh yield and fracture strength for $\langle 111 \rangle$ oriented single crystalline Au nanowires by quantitative *in situ* tensile experiments. In their experiment, one end of the short nanowires is adhered onto a gold or tungsten scanning tunneling microscope probe using conductive silver glue and the other end is attached to the tip of the silicon AFM cantilever with a thin adhesive layer of nanoscale amorphous silica. Here, the enhanced strength introduced by the hard silica layer can be one of the sources of the observed ultrahigh yield and fracture strength. While the direct and

FIG. 6. Sketch of hard/soft/hard sandwich structured nanowire.

FIG. 7. Atomic model of Cu/Al/Cu sandwich structured nanowire.

systematical experimental evidences are still lacking, more experiments are needed to verify the present results and realize the opinion.

In order to corroborate the high-strength and high-elongation of the ultrashort nanowires induced by the fixed ends, a Cu/Al/Cu sandwich structured nanowire, as shown in Fig. 7, is modeled using the molecular dynamics with an embedded atom-method potential.³⁷ In this sandwich structured nanowire, the initial length and diameter are 7.01 nm and 6.61 nm for the middle part ultrashort Al nanowire and 7.01 nm and 9.26 nm for the Cu nanowires located at the two ends, respectively. The end faces of Cu nanowires with (100) surface and Al nanowires with (111) surface are joined in the present model. The resulted stress-strain curve of this sandwich structured nanowires is compared with Al nanowires (with length 42.09 nm, diameter 6.61 nm) in Fig. 8. The impressively high elongation $\sim 325.01\%$ of the sandwich structured nanowires is considerably larger than the elongation $\sim 46.50\%$ of the Al nanowires. However, the strength of the sandwich structured nanowire is not strengthened compared with the Al nanowires. Here, the Cu-Al interface is strong enough to block the development of dislocations and confine all the plastic deformation within the region of Al, as shown in Fig. 9(b). The dislocation motion constrained by the Cu-Al interface facilitates the uniform deformation along the length of the middle part Al nanowires, and postpones the occurring of necking, as shown in Fig. 9(c). Hence,

FIG. 8. The engineering stress-strain curves for Cu/Al/Cu sandwich structured nanowire and Al nanowire.

FIG. 9. Snapshot of the plastic deformation of Cu/Al/Cu sandwich structured nanowire. (a) $\varepsilon = 11.50\%$, the first partial dislocation nucleates; (b) $\varepsilon = 100\%$, the dislocations are blocked by the interface; (c) $\varepsilon = 325\%$, the fracture morphology.

the high elongation is captured by the Cu/Al/Cu sandwich structured nanowire. While the interface has no effect on the nucleation of first partial dislocation, as shown in Fig. 9(a), there is no enhanced strength. In the previous simulation, the fixed layer has the coherent interface with the nanowires, while the Cu-Al interface is not coherent. Recently, an enhanced strength imported by the coherent twin boundary has been generally accepted.^{38,39} So, we predict that the atomic structure of interface is responsible for the missing enhanced strength in the present Cu/Al/Cu sandwich structured nanowires.

In summary, the Cu/Al/Cu sandwich structured nanowires can be realizable in experimental to verify the unique properties of ultrashort nanowires discovered in our molecular dynamics simulations. And it suggests a new approach to strengthen and toughen the nanowires. The molecular dynamics simulation supplies a preliminary evidence to support the present prediction. The further and systematic molecular dynamics simulations should be studied to verify the results under a large deformation condition, and focus on interface structure and its effect on the mechanical properties to get a detailed investigation of the sandwich structured nanowires.

V. CONCLUSIONS

In summary, the uniaxial tensile behaviors of the single crystal Au $\langle 111 \rangle$ nanowires are studied using large-scale molecular dynamics simulation. The results indicate that the ultrashort nanowires ($L < L_{min}$) exhibit a unique combination of high strength and high elongation. We attribute the high elongation to the constrained dislocations motions characterized by the transient slipping of a large number of dislocations at multiple distinct slip system. The occurrence of high elongation is dominated by whether the deformation can spread the entail length, and the high strength is leaded by the constrained partial dislocation nucleation. A mechanical model based on image force theory is developed to provide an insight to dislocation nucleation and to capture the yield strength and nucleation site of first partial dislocation indi-

cated by simulation results. The model predictions are in excellent agreement with the simulation results.

Inspired by the superior properties of ultrashort nanowires, we suggest a new approach to strengthen and toughen nanowires-hard/soft/hard sandwich structured nanowires. A preliminary evidence from the molecular dynamics simulation supports this opinion. The sandwich structured nanowires also provide a possible experimental method to verify the unique properties of ultrashort nanowires discovered by the molecular dynamics simulation.

Until now, the deformation and failure mechanisms of the Au nanowires depending on the length are mapped in detail. The yield strength and elongation all decrease with increasing the length. The transition of two failure modes occurs with increasing the nanowires length. The ultrashort nanowires ($L < L_{min}$) expose high-elongation and high-strength, and fail via constrained dislocation plasticity along the multiple slip planes; the superlong nanowires ($L > L_c$) reveal brittle failure caused by an unstable localized shear along a single slip plane. While the intermediate-long nanowires ($L_{min} < L < L_c$) exhibit the ductile failure via the emergence of free dislocation plasticity along multiple slip planes. The present work suggests an understanding of engineering principles in designing the nanoscale devices.

ACKNOWLEDGMENTS

The authors acknowledge support by the National Natural Science Foundation of China (51075318), and Natural Science Foundation of Shannxi Province, China (2010JM6011).

- ¹C. Wang, Y. J. Hu, C. M. Lieber, and S. H. Sun, *J. Am. Chem. Soc.* **130**, 8902 (2008).
- ²W. Lu and C. M. Lieber, *Nature Mater.* **6**, 841–850 (2007).
- ³M. D. Uchic, D. M. Dimiduk, J. N. Florando, and W. D. Nix, *Science* **305**, 986–989 (2004).
- ⁴J. R. Greer, W. C. Oliver, and W. D. Nix, *Acta Mater.* **53**, 1821–1830 (2005).
- ⁵S. Brinckmann, J. Kim, and J. R. Greer, *Phys. Rev. Lett.* **100**, 155502 (2008).
- ⁶J. P. L. J. Hirth, *Theory of Dislocations* (John Wiley & Sons, New York, 1982).
- ⁷H. Tang, K. W. Schwarz, and H. D. Espinosa, *Phys. Rev. Lett.* **100**, 185503 (2008).
- ⁸T. Zhu, J. Li, A. Samanta, A. Leach, and K. Gall, *Phys. Rev. Lett.* **100**, 025502 (2008).
- ⁹A. T. Jennings, J. Li, and J. R. Greer, *Acta Mater.* **59**, 5627–5637 (2011).
- ¹⁰A. M. Leach, M. McDowell, and K. Gall, *Adv. Funct. Mater.* **17**, 43–53 (2007).
- ¹¹K. Gall, J. Diao, and M. L. Dunn, *Nano Lett.* **4**, 2431–2436 (2004).
- ¹²E. Rabkin, H. S. Nam, and D. J. Srolovitz, *Acta Mater.* **55**, 2085–2099 (2007).
- ¹³A. Cao and E. Ma, *Acta Mater.* **56**, 4816–4828 (2008).
- ¹⁴C. R. Weinberger, A. T. Jennings, K. Kang, and J. R. Greer, *J. Mech. Phys. Solids* **60**, 84–103 (2011).
- ¹⁵J. Y. Kim and J. R. Greer, *Acta Mater.* **57**, 5245–5253 (2009).
- ¹⁶D. Kiener, W. Grosinger, G. Dehm, and R. Pippan, *Acta Mater.* **56**, 580–592 (2008).
- ¹⁷A. T. Jennings and J. R. Greer, *Philos. Mag.* **91**, 1108–1120 (2011).
- ¹⁸G. Richter, K. Hillerich, D. S. Gianola, R. Mönnig, O. Kraft, and C. A. Volkert, *Nano Lett.* **9**, 3048–3052 (2009).
- ¹⁹Y. Lu, J. Song, J. Y. Huang, and J. Lou, *Adv. Funct. Mater.* **21**, 3982–3989 (2011).
- ²⁰Z. Wu, Y. Zhang, M. H. Jhon, H. Gao, and D. J. Srolovitz, *Nano Lett.* **12**, 910–914 (2012).

- ²¹G. Grochola, S. P. Russo, and I. K. Snook, *J. Chem. Phys.* **123**, 204719 (2005).
- ²²S. Ryu, K. Kang, and W. Cai, *J. Mater. Res.* **26**, 2335–2354 (2011).
- ²³T. Schneider and E. Stoll, *Phys. Rev. B* **17**, 1302–1322 (1978).
- ²⁴S. J. A. Koh and H. P. Lee, *Nanotechnology* **17**, 3451–3467 (2006).
- ²⁵S. Nose, *J. Chem. Phys.* **81**, 511–519 (1984).
- ²⁶W. G. Hoover, *Phys. Rev. A* **34**, 2499–2500 (1986).
- ²⁷H. Tsuzuki, P. S. Branicio, and J. P. Rino, *Comput. Phys. Commun.* **177**, 518–523 (2007).
- ²⁸J. D. Honeycutt and H. C. Andersen, *J. Phys. Chem.* **91**, 4950–4963 (1987).
- ²⁹A. Rinaldi, P. Peralta, C. Friesen, D. Nahar, S. Licoccia, E. Traversa, and K. Sieradzki, *Small* **6**, 528–536 (2010).
- ³⁰Z. S. Pereira and E. Z. Da Silva, *J. Phys. Chem. C* **115**, 22870–22876 (2011).
- ³¹Y. Lu, J. Y. Huang, C. Wang, S. Sun, and J. Lou, *Nat. Nanotechnol.* **5**, 218–224 (2010).
- ³²S. H. Oh, M. Legros, D. Kiener, and G. Dehm, *Nature Mater.* **8**, 95–100 (2009).
- ³³C. Vieu, F. Carcenac, A. Pepin, Y. Chen, M. Mejias, A. Lebib, L. Manin-Ferlazzo, L. Couraud, and H. Launois, *Appl. Surf. Sci.* **164**, 111–117 (2000).
- ³⁴A. Misra, J. P. Hirth, and H. Kung, *Philos. Mag. A* **82**, 2935–2951 (2002).
- ³⁵D. E. Kramer and T. Foecke, *Philos. Mag. A* **82**, 3375–3381 (2002).
- ³⁶Y. Lu, J. Song, J. Y. Huang, and J. Lou, *Nano Res.* **4**, 1261–1267 (2011).
- ³⁷J. Cai and Y. Y. Ye, *Phys. Rev. B* **54**, 8398–8410 (1996).
- ³⁸L. Lu, Y. F. Shen, X. H. Chen, L. H. Qian, and K. Lu, *Science* **304**, 422–426 (2004).
- ³⁹D. Jang, X. Li, H. Gao, and J. R. Greer, *Nat. Nanotechnol.* **7**, 594 (2012).