Atomistic Simulations of Compression Tests on Ni$_3$Al Nanocubes

J. Amodeo$^a$, C. Begau$^b$ and E. Bitzek$^a$*

$^a$Department of Materials Science and Engineering, Institute of General Material Properties (WW1), Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), Martensstrasse 5, 91058 Erlangen, Germany; $^b$Interdisciplinary Centre for Advanced Materials Simulation (ICAMS), Ruhr-Universität Bochum (RUB), 44801 Bochum, Germany

(Received 4 November 2013; final form 21 December 2013)

Supplementary Material Available Online

The deformation behaviour of nano-sized Ni$_3$Al cubes with $\{100\}$ side surfaces is investigated under uniaxial compression using constant-temperature molecular dynamics simulations at 300 K. The simulations reproduce key features of recently performed nanocompression experiments, namely the lack of strain hardening, homogeneous deformation of the entire sample and overall high stress levels of the order of 3–5 GPa. According to the simulations, the critical initial step is the formation of a pseudo-twin structure, which then further deforms by Shockley partial dislocations. These deformation mechanisms differ significantly from bulk Ni$_3$Al and are rationalized in terms of generalized stacking fault energies and resolved shear stresses.

Keywords: Small-Scale Plasticity, MD Simulations, Ni$_3$Al, Dislocations, Twinning

1. Introduction

Nanometer-sized metallic structures such as nanopillars, nanowires (NWs), nanoparticles and thin films have attracted substantial interest due to their special mechanical behaviour: they generally show an increased yield strength compared with the bulk material as well as a size-dependent elastic response.[1–4] Whereas the size effect in the elastic constants is commonly attributed to a combination of surface stress effects and nonlinear elasticity,[1,2] the general trend of ‘smaller is stronger’ currently lacks an explanation in terms of a unified plasticity theory.[4] Several mechanisms leading to this trend have been suggested, including dislocation source truncation and source exhaustion, dislocation starvation and nucleation-controlled plasticity.[3,4] Furthermore, the nature of dislocation-based elementary mechanisms itself may become size-dependent at the nanoscale, where plasticity based on partial dislocations and deformation twinning (DT) can replace bulk-like ordinary dislocation plasticity (ODP).[3,5–9] Most of the studies on small-scale plasticity were performed on face centered cubic (fcc) metals. Only recently more work on body centered cubic (bcc), hexagonally closed packed (hcp) and more complex alloys is being performed.[7,10,11]

Last year, two research groups used a wet-chemical process to extract 200–600 nm sized cubic precipitates from the $\gamma/\gamma'$-microstructure of a Ni-based superalloy (CMSX-4) to perform nanocompression tests.[12–14] After standard heat treatment, the precipitates do not contain dislocations, and the wet-chemical route precludes the creation of defects in $\gamma'$-Ni$_3$Al cubes ($L_1_2$ crystallographic structure). Contrary to samples prepared by focussed ion-beam (FIB) milling, these free-standing nanocubes are free of dislocations.[15] Room temperature (RT) compression tests on these defect-free nanocubes show high-yield stresses up to a substantial portion of the theoretical strength, large strain bursts and homogeneous deformation for engineering strains up to 100% without signs of particle damage.[12–14] It is well established that RT deformation of bulk-Ni$_3$Al takes place by $\{110\}|\{111\}$ superdislocations, which can include the formation of planar defects like complex stacking faults (CSF), anti-phase boundary (APB) or super intrinsic stacking fault.[16,17] Whether these superdislocations also carry the plastic deformation during the compression of the Ni$_3$Al nanocubes, or whether a change in deformation mechanism like, e.g. in pristine fcc NWs [8,9] takes place has so far not been studied.

*Corresponding author. Email: erik.bitzek@fau.de

© 2014 The Author(s). Published by Taylor & Francis. This is an Open Access article distributed under the terms of the Creative Commons Attribution License (http://creativecommons.org/licenses/by/3.0), which permits unrestricted use, distribution, and reproduction in any medium, provided the original work is properly cited. The moral rights of the named author(s) have been asserted.
2. Computational Methods

In this study, we performed molecular dynamics (MD) simulations to investigate the deformation mechanisms of initially defect-free Ni₃Al nanocubes under compression at RT. We used the embedded-atom method potential for the Ni/Ni₃Al systems developed by Mishin,[18] which represents well the equilibrium properties and defect energies of the γ’-phase (see the supplementary material at http://dx.doi.org/10.1080/21663831.2013.878884 for details of the potential properties and the choice of the potential). Cubic samples with 10 and 25 nm edge lengths were modelled with free surfaces oriented along the (100) directions.

After structural optimization with the FIRE algorithm,[19] the samples were equilibrated for 25 ps at 300 K using standard MD followed by 100 ps using the Nosé–Hoover thermostat.[20] Compression tests were performed using two external potentials which model the flat punch indenter and the substrate. The potential form was adapted from Van Vliet et al. [21] using as parameters $r_{\text{cut}} = 5\, \text{Å}$ and $d = 0.8$. To model uniaxial compression along the [001] direction, the top indenter was subjected to a constant displacement rate of 0.011 and 0.025 Å/ps, respectively, for the 11 and the 25 nm sized cubes, which corresponds to a strain rate of $10^8\, \text{s}^{-1}$. The bottom potential was kept fixed. During the compression tests, a time step of 2 fs was used and a temperature of 300 K was imposed using the Nosé–Hoover thermostat.

The simulations results were analyzed using AtomViewer.[22] For our purpose, a modified version of the bond-angle analysis [23] with the capability to identify crystalline structures and complex stacking faults inherent to Ni₃Al was implemented. Furthermore, this tool combines Nye-tensor analysis for Burgers vector identification [24,25] and dislocation skeletonization.[26] For complementary analysis, the centrosymmetry parameter (CSP) as well as the coordination number for binary systems were used. See the supplementary material at http://dx.doi.org/10.1080/21663831.2013.878884 for more details on the analysis methods.

3. Results

Both samples were deformed up to a true strain of $\varepsilon = 3\%$. As shown in Figure 1, the stress–strain curves for both sample sizes are comparable to each other and can be divided into three regimes of deformation (referenced later as Stages 1, 2 and 3). As the fundamental deformation mechanisms in both cubes are identical, we in the following only present the analysis for the 11 nm sample. Additional simulations with different initial velocities and lower strain rates were performed and showed no significant differences (see the supplementary material at http://dx.doi.org/10.1080/21663831.2013.878884).

After the contact between the sample and the indenter is established, the cube starts to deform elastically. Up to $\varepsilon = 3\%$, the stress increases linearly with strain according to a Young’s modulus of $E = 80.2\, \text{GPa}$ ($E = 86.7\, \text{GPa}$ for the 25 nm sample). These values are significantly lower than the Young’s modulus in (100)-direction determined from the elastic constants of the potential $E_{(100)} = 114.1\, \text{GPa}$. This is an example for the well-known size dependence of elastic constants in nanoparticles, see, e.g. [1,2,27] and the supplementary material at http://dx.doi.org/10.1080/21663831.2013.878884. At higher strains, the stress response is nonlinear and the stress decreases after reaching a maximum of about 3.9 GPa. A similar behaviour was recently reported by Wang et al.[27] who used density functional theory to study the elastic response of bulk Ni₃Al under tension along the [100]-axis. They also studied in detail the decrease in the Young’s modulus with decreasing diameter in atomistic simulations of [100]-oriented single crystalline Ni₃Al NWs, which is attributed to the presence of surface stresses and anharmonic elasticity.[27] We will therefore focus in the following on the plastic deformation mechanisms of the Ni₃Al cubes rather than on their elastic response.

The first evidence of plastic deformation occurs at $\varepsilon = 10.1\%$ and a true stress of about $\sigma = 3.8\, \text{GPa}$ when a dislocation is nucleated at an edge of the cube, see Figure 2(a). The Burgers vector of the dislocation is $\vec{b} = \frac{1}{6}[1\bar{1}2]$, which corresponds to a Shockley partial dislocation. The glide plane of the dislocation is the (111) plane, on which it creates a CSF. Further partial dislocations with same Burgers vector and glide plane are nucleated between $\varepsilon = 10.1\%$ and $\varepsilon = 14.0\%$ on parallel planes in the vicinity of the first partial dislocation. The dislocations are each spaced four atomic planes apart, which leads to a regular stacking of CSFs every $4n$ planes, see Figure 2(b). The dislocations assume their stable equilibrium position on top of each other rather than gliding through the entire cube. At $\varepsilon = 14.0\%$, multiple $\frac{1}{6}[1\bar{1}2](1\bar{1}1)$ partial dislocations suddenly nucleate.
AC is changed according to the space group C2/m and the stacking sequence (Figure 1). Bands in which the CSF are spaced 2 is reflected in the sudden increase in the contact area \( \bar{\varepsilon} \) atomic (\( \bar{\varepsilon} \)).

From elastic reloading during which no new defects occur.

The nanocompression experiments reported in the literature were performed at strain rates of the order of \( 10^{-3} \) s\(^{-1} \) on \( \gamma' \)-cubes extracted from the CMSX-4 alloy with side lengths between 200 and 600 nm.[12–14] Despite the differences in size, strain rate and composition, our simulation results reproduce some of the key features of the experiments, namely the lack of strain hardening which is a prerequisite for the observed large strain bursts, homogeneous deformation of the entire sample with slip steps on the surfaces rather than localized slip as in the case of FIB-irradiated \( \gamma' \)-cubes,[13] and overall high stress levels of the order of 3–5 GPa.[12–14]

4. Discussion

The beginning of Stage 2 is characterized by an elastic reloading during which no new defects occur. From \( \varepsilon = 19.6\% \) on, additional \( \frac{1}{6} [112] \) partial dislocations are emitted (Figure 3(a)), which lead to the stress drop in Figure 1. The stacking faults left behind by these dislocations are characterized by lower CSP and higher potential energy than those that had been observed during Stage 1. The partial dislocations start to fill the \( \bar{\varepsilon} \) -cubes forming large bands (Figure 3(b)). The crystal structure within these bands corresponds to the pseudo-twin structure.[28] In this case, the structure is obtained by shearing the previous CSF multistack by \( \frac{1}{6} [112] \) every \( 2n + 1 \) \( [111] \) planes, i.e. in between the already present CSF. Therefore, the stacking sequence changes from \( \ldots AC'AC'AC'AC' \ldots \) to \( \ldots AC'BA'CB'AC'B \ldots \).

This stacking sequence differs only slightly from the \( L_12 \) true-twin structure \( \ldots ACBACBACB \ldots \) which requires thermally activated reordering between Ni an Al atoms.[28,29] At the end of Stage 2, the entire sample was transformed to the pseudo-twin structure, resulting in a more prolate parallelepiped shape.

The onset of Stage 3 is characterized by an elastic reloading which involves an increase in the true stress to the maximum value of about 8 GPa. At \( \varepsilon = 31.8\% \), multiple partial dislocations are nucleated within the pseudo-twin structure from the edges and the top surface. Slip takes place on the \( [111] \) and \( [111] \) planes (in the pseudo-twin coordinate system), see Figure 3(c). Large slip steps are produced by the subsequent slip of multiple dislocations on the same slip plane. These dislocations produced stacking faults which in the bond-angle analysis have the signature of CSFs and APBs. While Stages 1 and 2 were characterized by the highly correlated motion of partial dislocations, Stage 3 is clearly governed by ODP.
The deformation behaviour and strain bursts observed in the experiments were attributed to the initial lack of dislocations within the γ’-cubes which allows the sample to sustain large stresses close to the theoretical strength at which finally ‘explosive dislocation nucleation’ occurs [13] or an ‘avalanche-like’; deformation process sets in [14].

Based on our simulation results, we suggest an alternative deformation scenario, in which the critical initial step is the formation of a pseudo-twin structure, which then further deforms by ODP. Deformation by pseudo-twinning has also been recently reported in MD simulations of Ni₃Al samples subjected to high stresses.[27,30] We assume that even under the experimental conditions during nanocompression tests,[12–14] pseudo-twinning rather than twinning can be expected, as the latter involves thermally activated reordering processes. The critical migration barrier for this process has been determined to be ~0.93 eV,[29] which at RT makes this process very unlikely to massively occur during the sub-second displacement bursts.

In the case of initially dislocation-free samples, the yield stress for deformation by pseudo-twinning has to be identical to the one in the case of ODP because the first step in both processes is the nucleation of a leading partial dislocation. However, in the experiments, the fast, highly correlated, ‘laser-like’,[7] dislocation motion during pseudo-twinning would significantly reduce the possibility for their interaction with each other or with stacking faults compared with the more chaotic ODP. Thus, pseudo-twinning seems a natural alternative to the ‘avalanche-like’ ODP-processes proposed in [14] to explain the lack of strain hardening and the instability causing the strain burst in the closed-loop displacement-controlled experiments of γ’ nanocube compression.[13] In the following we will show that pseudo-twinning is furthermore the energetically favoured initial deformation mechanism.

Twinning is frequently observed in single-crystalline fcc NWs, where it strongly depends on the orientation, the diameter and the orientation of the side surfaces, see, e.g. the recent review by Weinberger and Cai.[9] The competition between slip and twinning in fcc NWs is usually discussed in the framework of the generalized stacking fault (GSF) energy surface.[9,31] The gist of this reasoning in fcc metals can be applied to the L₁₂ structure, however with the important difference that one needs to consider the various planar fault energies and the existence of superdislocations. Figure 4 shows 1D-GSF energy profiles along the relevant ⟨112⟩ and ⟨110⟩ directions on the ⟨111⟩ planes (see supplementary material at http://dx.doi.org/10.1080/21663831.2013.878884 for details on the calculation method). The displacements are normalized by the 1/6⟨112⟩ Burgers vectors required to create the corresponding stacking faults (CSF, APB, pseudo-twins, etc.). From this figure, it can be seen that the energy of an APB is lower than the energy of two CSFs (252.0 and 394.2 mJ/m², respectively). Therefore, it is energetically favourable for plastic deformation to take place by 1/6⟨110⟩ superpartial dislocations bounded by an APB rather than by individual Shockley partial dislocations leaving behind CSFs. However, from a kinetic point of view, the energy barrier along this path is only slightly higher than for the creation of 2 CSF, see Figure 4. Both processes could therefore take place with about the same probability. However, taking into account only the energy barriers as described by the GSF curves, neglects the work done on the dislocation by the applied stress:[8,9] under uniaxial compression along the [001] direction, the Schmid factor m = 0.471 for the leading partial dislocation 1/6⟨112⟩⟨111⟩ is two times higher than for the trailing partial dislocations 1/4⟨121⟩⟨111⟩ or 1/2[211]⟨111⟩ (m = 0.236). As the energy barriers related to the creation of APBs or CSFs are comparable, the nucleation of further leading dislocations rather than of trailing partial dislocations is significantly favoured by the compressive stress, even though this entails the creation of further CSFs rather than APBs.

In contrast to twinning in monoatomic fcc metals, the energy of a pseudo-twin in the L₁₂ structure is proportional to the number of its atomic layers n. This is due to the formation of Al–Al and Ni–Ni forbidden bonds with each additional pseudo-twin plane. Figure 4 shows that the energy of n parallel CSFs produced by leading partial dislocations with identical Burgers vector in every second plane is lower than for a n-layer pseudo-twin. This explains why the pseudo-twin was formed in a two-step process (Stages 1 + 2): only after the sample is entirely filled with parallel CSFs every two planes,
further shear by the same Burgers vector with maximal Schmid factor will take place on the planes between the CSFs, transforming the structure into a pseudo-twin. This is an important difference to twinning in fcc metals: there, nanotwins can directly form on top of a stacking fault, and once a nanotwin has been formed, the nucleation stress for twinning dislocations is lower than for the leading partial dislocation as the twin boundary is only propagated by one atomic layer and no new fault is formed. In the L12 structure, the nucleation of a twinning dislocation requires a higher stress (Stage 2) than the initial partial dislocation (Stage 1), and depends on the internal structure of the sample (CSFs on every second plane).

Although the deformation mechanisms discussed here were gleaned from MD simulations at high strain rates, the above discussion is purely based on energy arguments. Whereas the yield stress is clearly influenced by the strain rate dependence of dislocation nucleation from the corners, see [32], the importance of pseudo-twinning during the compression of γ′-nanocubes is therefore most probably largely independent of the strain rate.

Our simulation results show that similar to monoatomic fcc metals,[5,8,9] the deformation mechanisms in Ni3Al can change with decreasing sample size from ODP to DT, and the same arguments can be used to explain this size effect: DT at RT requires the absence of competing dislocation processes and the formation of stacking faults as the initial step. Small samples are often dislocation free, and thus require high stresses to nucleate dislocations.[3,4,33] Whether partial or full dislocations are nucleated depends on the size of the dislocation source, which scales with the sample size.[5,8] The critical size at which partial dislocation activity and twinning are observed to take over ODP is of the order of hundreds of nanometers,[3] with typical dislocation source sizes of $D_c \approx 40\,\text{nm}$. [8] Adapting the approach of Chen et al.[5,8] the critical source size at which the formation of superdislocations rather than partial dislocations is favoured can be estimated to $D_c \approx 50\,\text{nm}$ (see supplementary material at http://dx.doi.org/10.1080/21663831.2013.878884). It can be therefore assumed that, similar to the situation in [8], the experimentally used cube sizes of 200–600 nm lie within the size range in which pseudo-twinning can be expected. For cube sizes below 5 nm, however, surface stress effects are expected to dominate,[9,27,34,35] and a transition of deformation mechanism to phase transformations might take place.[27]

The situation is different in Ni-based superalloys, where the γ′-Ni3Al cubes form the strengthening phase.[36] There, γ′-precipitates deform typically by glide of superdislocations which are formed by pairs of $\frac{1}{2}(110)$ dislocations from the γ-matrix channels.[17,37] However, recently the formation of microtwins which shear both the matrix and the precipitates has been reported as a critical deformation mechanism during creep experiments at intermediate temperatures.[29,38] Understanding the underlying mechanisms leading to twinning of the γ/γ′-microstructure requires detailed knowledge about the processes during (pseudo-) twinning in the constituting phases. Future experiments and simulations of nanocompression tests on γ′-nanocubes at different temperatures could provide important complementary information on the natural deformation mechanisms of γ′-precipitates which could be used, e.g., in mesoscopic models for creep in superalloys.[39]

5. Conclusion In summary, MD simulations of RT compression test on nano-sized Ni3Al cubes reproduced some of the key features of the corresponding experiments.[12–14] The results suggest that the initial deformation takes place by pseudo-twinning rather than ODP, which also can explain the experimentally observed strain bursts. Analysis of the GSF energy curves and the resolved shear stresses furthermore shows that pseudo-twinning is also the energetically favoured deformation mechanism. The process of pseudo-twinning is structurally different from twinning in fcc metals and takes place in two steps, where the final twinning dislocations require a higher stress than the initial partial dislocations. Whether pseudo-twinning is also relevant during nanocompression experiments on larger cubes, with different compositions and at lower strain rates than in the simulations should be easily verifiable (or falsifiable) by transmission electron microscopy analysis of compressed γ′-cubes.

6. Supplementary online material A more detailed information on the simulations is available at http://dx.doi.org/10.1080/21663831.2013.878884.

Acknowledgements The authors acknowledge support by the Deutsche Forschungsgemeinschaft (DFG) through project C3 of SFB/Transregio 103 (Single Crystal Superalloys).

References
[1] Liang H, Upmanyu M, Huang H. Size-dependent elasticity of nanowires: nonlinear effects. Phys Rev B. 2005;71(24):241403.
[2] McDowell M, Leach A, Gall K. On the elastic modulus of metallic nanowires. Nano Lett. 2008;8(11):3613–3618.
[3] Kraft O, Gruber P, Mönig R, Weygand D. Plasticity in confined dimensions. Ann Rev Mater Res. 2010;40:293–317.
[4] Greer J, De Hosson J. Plasticity in small-sized metallic systems: intrinsic versus extrinsic size effect. Progr Mater Sci 2011;56(6):654–724.
[5] Chen M, Ma E, Hemker K, Sheng H, Wang Y, Cheng X. Deformation twinning in nanocrystalline aluminum. Science. 2003;300(5623):1275–1277.
[6] Oh S, Legros M, Kiener D, Gruber P, Dehm G. In situ TEM straining of single crystal Au films on polyimide: change
of deformation mechanisms at the nanoscale. Acta Mater. 2007;55(16):5558–5571.
[7] Yu Q, Shan ZW, Li J, Huang X, Xiao L, Sun J, Ma E. Strong crystal size effect on deformation twinning. Nature. 2010;463(7279):335–338.
[8] Sedlmayr A, Bitzek E, Gianola D, Richter G, Mönig R, Kraft O. Existence of two twinning-mediated plastic deformation modes in Au nanowhiskers. Acta Mater. 2012;60(9):3985–3993.
[9] Weinberger CR, Cai W. Plasticity of metal nanowires. J Mater Chem. 2012;22(8):3277–3292.
[10] Korte S, Stearn RJ, Wheeler JM, Clegg WJ. High temperature microcompression and nanoindentation in vacuum. J Mater Res. 2011;27(1):167–176.
[11] Withey E, Minor A, Chrzan D, Morris J, Kuramoto S. The deformation of Gum Metal through in situ compression of nanopillars. Acta Mater. 2010;58(7):2652–2665.
[12] Schloesser J, Roesler J, Mukherji D. Deformation behaviour of freestanding single-crystalline Ni3Al-based nanoparticles. Int J Mater Res. 2011;102(5):532–537.
[13] Maåb R, Meza L, Gan B, Tin S, Greer J. Ultrahigh strength of dislocation-free Ni3Al nanocubes. Small. 2012;8(12):1869–1875.
[14] Landefeld A, Mook WM, Rösler J, Michler J. Compression experiments on γ′-nanoparticles. ISRN Nanomater. 2012;2012:1–4.
[15] Mukherji D, Müller R, Gilles R, Strunz P, Rösler J. Nanocrystalline Ni3Al-type intermetallic phase powder from Ni-base superalloys. Nanotechnology. 2004;15(5):648–657.
[16] Kear B, Oblak J, Giamai C. Stacking faults in gamma prime Ni3Al(Ti) precipitation hardened nickel-base alloys. Metal Mater Trans B. 1970;1(9):2477–2486.
[17] Pope D, Ezzi S. Mechanical properties of NiAl and nickel-base alloys with high volume fraction of γ′. Int Metal Rev. 1984;29(1):136–167.
[18] Mishin Y. Atomistic modeling of the χ and χ′-phases of the Ni–Al system. Acta Mater. 2004;52(6):1451–1467.
[19] Bitzek E, Koskinen P, Gähler F, Moseler M. Structural relaxation made simple. Phys Rev Lett. 2006;97:170201.
[20] Hoover W. Canonical dynamics: equilibrium phase-space distributions. Phys Rev A. 1985;31(3):1695.
[21] Van Vliet K, Li J, Zhu T, Yip S, Suresh S. Quantifying the strength of dislocation-free Ni3Al nanocubes. Small. 2012;8(12):1869–1875.
[22] Begau C. AtomViewer. Available from: http://homepages.ruhr-uni-bochum.de/Christoph.Begau/
[23] Ackland G, Jones A. Applications of local crystal structure measures in experiment and simulation. Phys Rev B. 2006;73(5):054104.
[24] Hartley C, Mishin Y. Characterization and visualization of the lattice misfit associated with dislocation cores. Acta Mater. 2005;53(5):1313–1321.
[25] Begau C, Hua J, Hartmaier A. A novel approach to study dislocation density tensors and lattice rotation patterns in atomistic simulations. J Mech Phys Solids. 2012;60(4):711–722.
[26] Begau C, Hartmaier A, George EP, Pharr GM. Atomistic processes of dislocation generation and plastic deformation during nanoindentation. Acta Mater. 2011;59(3):934–942.
[27] Wang YJ, Gao G, Ogata S. Size-dependent transition of deformation mechanism, and nonlinear elasticity in Ni3Al nanowires. Appl Phys Lett. 2013;102:041902.
[28] Kolbe M. The high temperature decrease of the critical resolved shear stress in nickel-base superalloys. Mater Sci Eng A. 2001;319:383–387.
[29] Kovarik L, Unocic RR, Li J, Sarosi P, Shen C, Wang Y, Mills MJ. Microtwinning and other shearing mechanisms at intermediate temperatures in Ni-based superalloys. Progr Mater Sci. 2009;54(6):839–873.
[30] Xie HX, Bo L, Yu T. Atomistic simulation of microtwinning at the crack tip in L12 Ni3Al. Phil Mag. 2012;92(12):1542–1553.
[31] Vitek V. Intrinsic stacking faults in body-centred cubic crystals. Phil Mag. 1968;18(154):773–786.
[32] Zhu T, Li J, Samanta A, Leach A, Gall K. Temperature and strain-rate dependence of surface dislocation nucleation. Phys Rev Lett. 2008;100(2):025502.
[33] Mordehai D, Lee SW, Backes B, Srolovitz D, Nix W, Rabkin E. Size effect in compression of single-crystal gold microparticles. Acta Mater. 2011;59(13):5202–5215.
[34] Park H, Gall K, Zimmerman J. Shape memory and pseudoelasticity in metal nanowires. Phys Rev Lett. 2005;95(25):255504.
[35] Jiang JW, Leach AM, Gall K, Park HS. A surface stacking fault energy approach to predicting defect nucleation in surface-dominated nanostructures. J Mech Phys Solid. 2013;61(9):1915–1934.
[36] Reed R. The superalloys: fundamentals and applications. New York: Cambridge University Press; 2006.
[37] Pollock T, Field R. Dislocations and high-temperature plastic deformation of superalloy single crystals. In: Nabarro F, Duesbery M, editors. Dislocations in solids. Amsterdam, North-Holland: Elsevier; 2002. p. 547–618.
[38] Viswanathan G, Sarosi P, Henry M, Whits W, Mills M. Investigation of creep deformation mechanisms at intermediate temperatures in René 88 DT. Acta Mater. 2005;53(10):3041–3057.
[39] Haghighat S, Eggeler G, Raabe D. Effect of climb on dislocation mechanisms and creep rates in γ′-strengthened Ni base superalloy single crystals: a discrete dislocation dynamics study. Acta Mater. 2013;61:3709–3723.