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Atomistic Simulations of Compression Tests on Ni₃Al Nanocubes

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Supplementary Material Available Online

The deformation behaviour of nano-sized Ni₃Al 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 Ni₃Al and are rationalized in terms of generalized stacking fault energies and resolved shear stresses.

Keywords: Small-Scale Plasticity, MD Simulations, Ni₃Al, 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 γ/γ' -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 γ' -Ni₃Al cubes (L1₂ 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-Ni₃Al takes place by $\langle 110 \rangle \{111\}$ superdislocations, which can include the formation of planar defects like complex stacking faults (CSF), anti-phase boundary (APB) or superintrinsic stacking fault.[16,17] Whether these superdislocations also carry the plastic deformation during the compression of the Ni₃Al 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.

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2. Computational Methods In this study, we performed molecular dynamics (MD) simulations to investigate the deformation mechanisms of initially defect-free Ni_3Al nanocubes under compression at RT. We used the embedded-atom method potential for the $\text{Ni}/\text{Ni}_3\text{Al}$ 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 $\langle 100 \rangle$ 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 $r_{\text{cut}} = 5 \text{ \AA}$ 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 $\text{\AA}/\text{ps}$, respectively, for the 11 and the 25 nm sized cubes, which corresponds to a strain rate of 10^8 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 defects inherent to Ni_3Al 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 $\varepsilon = 38\%$. 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.

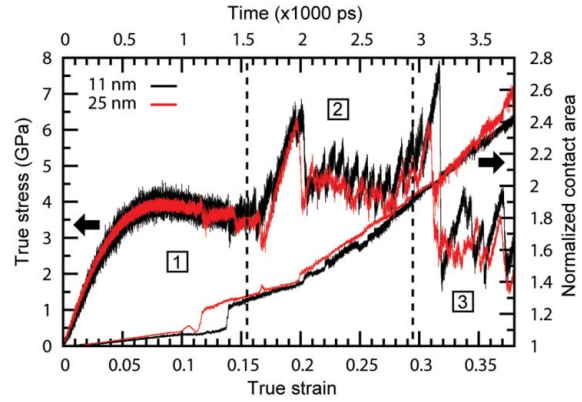


Figure 1. Stress–strain curves and evolution of normalized contact area for 11 nm (black) and 25 nm (red) cubes.

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 $\langle 100 \rangle$ -direction determined from the elastic constants of the potential $E_{\langle 100 \rangle} = 114.1 \text{ GPa}$. This is an example for the well-known size dependence of elastic constants in nano-objects, 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 Ni_3Al 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 Ni_3Al 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 Ni_3Al 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 $(\bar{1}11)$ 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 $\frac{1}{6}[1\bar{1}2](\bar{1}11)$ partial dislocations suddenly nucleate

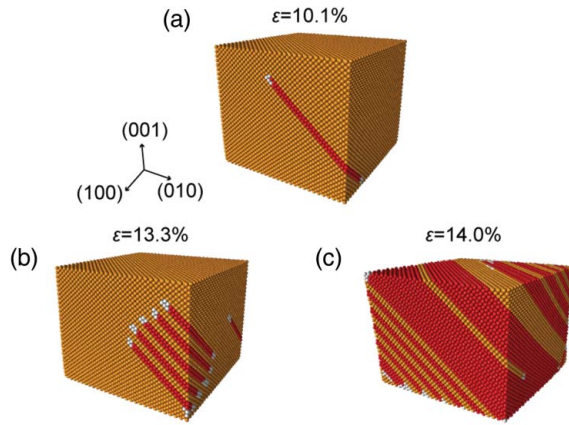


Figure 2. Dislocation activity during Stage 1 of deformation. Atoms coloured in orange and red represent the perfect $L1_2$ structure and CSF environment. Atoms in white refer to other defects, e.g. dislocation cores. For the sake of clarity, surface atoms have been removed.

and all dislocations propagate throughout the entire sample.

In this process, the sample shape starts to deviate from the original cubic shape and the aspect ratio decreases from 1/1 to about 4/5 (Figure 2), which is reflected in the sudden increase in the contact area (Figure 1). Bands in which the CSF are spaced $2n$ atomic ($\bar{1}\bar{1}1$) planes apart emerge, see Figure 2(c). The crystalline structure within these bands belongs to the space group $C2/m$ and the stacking sequence is changed according to $\dots ABCABCABC \dots \rightarrow \dots AC'A'CAC'A'CA \dots$ which is obtained by shearing the original structure of $\frac{1}{6}\langle 112 \rangle$ every $2n$ ($\bar{1}\bar{1}1$) planes.

This structure can be described as a hcp structure ($\dots CACACA \dots$ in the framework of monoatomic structures) made of hexagonal motifs with Al atoms at alternating positions every consecutive ($\bar{1}\bar{1}1$) planes. At the end of deformation Stage 1, the entire sample is transformed to this structure, and the shape corresponds now to a parallelepiped (see supplementary Figure S4 at <http://dx.doi.org/10.1080/21663831.2013.878884> for the evolution of the shape during the simulation).

The beginning of Stage 2 is characterized by an elastic reloading during which no new defects occur. From $\varepsilon = 19.6\%$ on, additional $\frac{1}{6}[1\bar{1}2](\bar{1}\bar{1}1)$ 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 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 $\frac{1}{6}\langle 112 \rangle$ every $2n + 1$ ($\bar{1}\bar{1}1$) planes, i.e. in between the already present CSF. Therefore, the stacking sequence changes

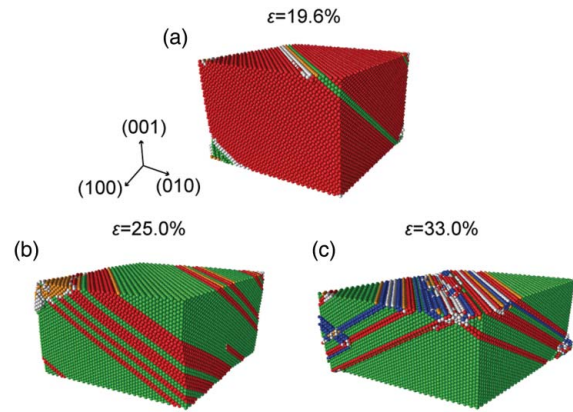


Figure 3. Dislocation activity during Stage 2(a), (b) and Stage 3(c). In addition to the colours in Figure 2, atoms coloured in green refer to the pseudo-twin structure, whereas atoms colored in blue belong to an APB environment. The coordinate system refers to the original orientation of the sample.

from $\dots AC'A'CAC'A'CA \dots$ to $\dots AC'BA'CB'AC'B \dots$. This stacking sequence differs only slightly from the $L1_2$ true-twin structure ($\dots ACBACBACB \dots$) which requires thermally activated reordering between Ni and 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 ($\bar{1}\bar{1}1$) and ($1\bar{1}1$) 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.

4. Discussion The nanocompression experiments reported in the literature were performed at strain rates of the order of 10^{-3} s^{-1} on γ' -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 γ' -cubes,[13] and overall high stress levels of the order of 3–5 GPa.[12–14]

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 Ni_3Al 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 metal 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 L_{12} 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 $\langle 112 \rangle$ and $\langle 110 \rangle$ 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 $\frac{1}{6}\langle 112 \rangle$ Burgers vectors required to create the corresponding stacking faults (CSF, APB,

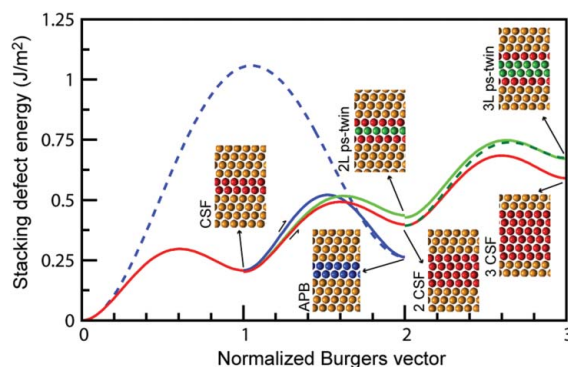


Figure 4. 1D Generalized stacking fault energy profiles for the $\langle 111 \rangle$ plane. The energy for rigid body displacements leading to one, two and three CSFs stacked on top of each other is plotted in red. The energy along the paths leading to an APB is in blue (solid line: energy path calculated for the displacements according to two $\langle 112 \rangle$ Shockley partial dislocations, dashed-line: direct displacement along the $[110]$ direction). Energy of paths leading to 2- and 3-layers pseudo-twin is in green.

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/m^2 , respectively). Therefore, it is energetically favourable for plastic deformation to take place by $\frac{1}{2}\langle 110 \rangle$ 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 $\frac{1}{6}[1\bar{1}2](\bar{1}11)$ is two times higher than for the trailing partial dislocations $\frac{1}{6}[1\bar{2}1](\bar{1}11)$ or $\frac{1}{6}[211](\bar{1}11)$ ($m = 0.236$). 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 L_{12} 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 $L1_2$ 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 Ni_3Al 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 critical dislocation source sizes of $D_c \approx 40$ 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 $D_c \approx 50$ 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' - Ni_3Al cubes form the strengthening phase.[36] There, γ' -precipitates deform typically by glide of superdislocations which are formed by pairs of $\frac{1}{2}\langle 110 \rangle$ 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 Ni_3Al 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>.

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