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Partial-mediated slips in nanocrystalline Ni at high strain rate

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Previous experiments on nanocrystalline Ni were conducted under quasistatic strain rates ($\sim 3 \times 10^{-3}$/s), which are much lower than that used in typical molecular dynamics simulations ($>3 \times 10^{7}$/s), thus making direct comparison of modeling and experiments very difficult. In this study, the split Hopkinson bar tests revealed that nanocrystalline Ni prefers twinning to extended partials, especially under higher strain rates (10^{3}/s). These observations contradict some reported molecular dynamics simulation results, where only extended partials, but no twins, were observed. The accuracy of the generalized planar fault energies is only partially responsible, but cannot fully account for such a difference. © *2007 American Institute of Physics*. [DOI: 10.1063/1.2745250]

To design nanocrystalline (nc) materials for superior mechanical properties, it is critical to understand their deformation physics.[1] Face-centered-cubic (fcc) nc metals have been reported to deform by partial dislocation emission from grain boundaries (GBs),[2–10] full dislocation,[3,5,7] GB sliding,[3,11–13] grain rotation,[11,14] and deformation twinning.[2,3,6–9,13–20] Significantly, recent molecular dynamics (MD) simulations (Ref. 5) as well as analytical models (Ref. 15) predicted that generalized planar fault energy (GPFE) curves play a critical role in the partial-dislocation-mediated slip in nc metals. Specifically, MD simulations predicted that nc Ni preferred to deform by extended partials despite its high stable stacking fault energy, and twinning was less favorable due to its very high unstable twin fault energy.[5] These results countered the conventional beliefs in the scientific community and stimulated more experimental work. To experimentally assess these MD simulation results, we recently deformed nc Ni film with an average grain size of 25 nm under tension at liquid nitrogen temperature.[20] Different than the MD prediction, both stacking faults and deformation twins were readily observed after deformation, with the density of twins higher than that of stacking faults. The observation of stacking faults agreed with the MD simulation prediction, however, the large number of twins contradicted it.

One of the major differences in experiments and MD simulations is the strain rates: the experiments were conducted under a quasistatic strain rate (3×10^{-3} s^{-1}), which is much lower than typical strain rates used in MD simulations ($>10^{7}$ s^{-1}).[3] Although high strain rates had been found to promote twinning in coarse-grained metals,[9,21] the huge difference in strain rates still raises an issue on the adequacy of the experimental results in validating MD simulation results. Therefore, it would be of interest to deform the nc Ni at a high strain rate and compare its deformation physics with that observed under the low strain rate and with MD simulation results. Another issue is the accuracy of the atomic potential used in MD simulations, which was found to significantly affect GPFE curves.[22] Recently, a more accurate GPFE curve for Ni was calculated from density function theory (DFT).[23] It would be of interest to analyze the experimental results along with the more accurate GPFE curve, since the GPFE curve determines the dominant deformation mechanisms in nc metals.

The objectives of this work were twofold: (1) to study the partial-dislocation-mediated slips in nc Ni at a high strain rate; and (2) to study the effect of the GPFE curves on its deformation physics. An electrodeposited nc-Ni foil with a thickness of 150 μm and an average grain size of $\sim$25 nm was purchased from Goodfellow Inc. Dynamic compression tests were carried out using a split Hopkinson pressure bar (SHPB) setup. Specimens of 8 mm in diameter were placed between an input bar and an output bar, each of them 8 mm in diameter and 2500 mm in length. The specimen and bars were immersed in liquid nitrogen. The input bar was impacted with a 3 kg projectile at a speed of $\sim$30 m/s. The specimen was deformed at a strain rate of $\sim 2.6 \times 10^{3}$ s^{-1}, which is much higher than that in previous experiments,[20] although still much lower than that in MD simulations.

We examined over 125 grains using high-resolution electron microscopy (HREM) and found grains containing twins, stacking faults, and full dislocations as well as "clean" grains (see Fig. 1). Figure 2 compares the fractions of grains containing different types of defects in samples deformed by SHPB tests and quasistatic tensile tests in the previous study.[20] For the SHPB tested sample, 44% of grains contain twins, while only 2% of grains contain stacking faults. This clearly indicates that twinning is the primary deformation mechanism at the high strain rate. Furthermore, comparing with the sample deformed under quasistatic strain rate, the high-strain-rate deformation doubled the fraction of grains containing twins while dramatically decreased the fraction of grains containing stacking faults from 16% to 2%. This in-

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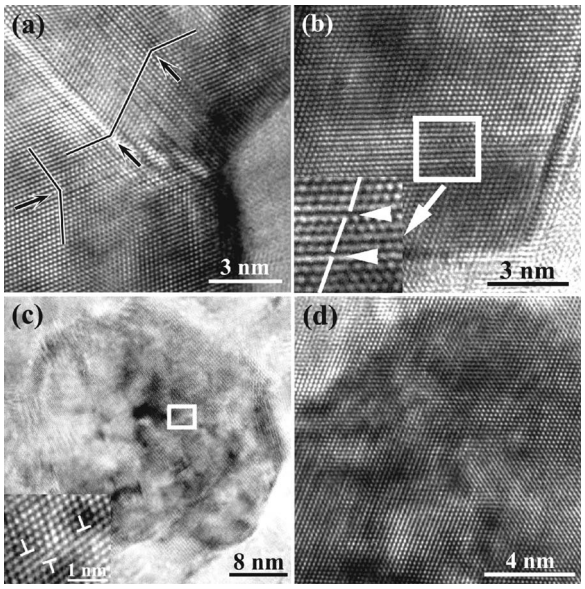

FIG. 1. HREM images of (a) multiple twins, (b) a stacking fault generated by an extended partial, (c) full dislocations, and (d) a grain free of defects in nc Ni deformed by split Hopkinson pressure bar (SHPB) tests at liquid nitrogen temperature.

dicates that deformation at high strain rates promotes deformation twinning. Therefore, it is most likely that at the extremely high strain rates used in MD simulations, more twins and less stacking faults will be observed than what is shown in Fig. 2. This strain rate effect on twinning propensity is consistent with that observed in coarse-grained metals.[21]

Samples deformed by both quasistatic tension and SHPB tests exhibited a significant fraction (40%–45%) of clean grains containing no twins, stacking faults, or dislocations. However, some of these clean grains might actually contain defects, but their orientation was such that HREM images did not reveal them. For example, the two {111} twinning planes in a twin can only be observed simultaneously along a particular ⟨110⟩ zone axis. However, there are six possible ⟨110⟩ axes in the fcc structure, making it easy to miss a twin if the grain is not oriented in the right orientation. Similar issues exist with the observation of stacking faults and dislocations. Therefore, the statistic over a large number of grains still can provide the overall trend of the role of each deformation mechanism.

To understand these experimental observations, we shall examine the GPFE curves, which have served as a basis for

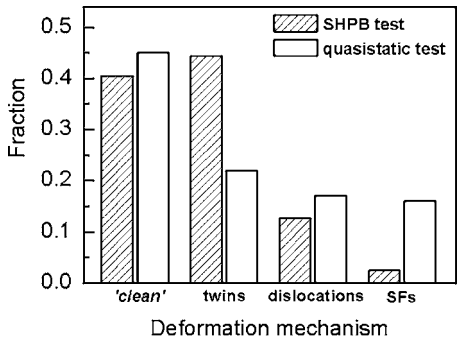

FIG. 2. Fractions of grains that contain different defect features in nc Ni samples deformed in liquid nitrogen by SHPB tests at a strain rate of $\sim 2.6\times 10^{3}\ s^{-1}$ and by quasistatic tensile tests at a strain rate of $3\times 10^{-3}\ s^{-1}$.

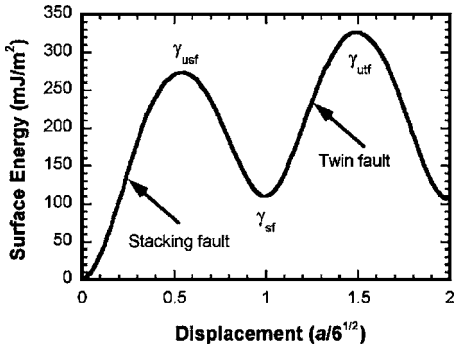

FIG. 3. Generalized planar fault energy (GPFE) curves for Ni calculated by the DFT (*ab initio*) approach. (see Ref. 23) γ_{sf} is the stable stacking fault energy; γ_{usf} is the unstable stacking fault energy; γ_{utf} is the unstable twin fault energy; a is the lattice constant.

the competing energetics to nucleate partials, full dislocations, or twins.[5] Extended partials were observed in MD simulations with the second moment tight binding potential of Cleri and Rosato for Ni.[24] But the value of GPFE curves changes dramatically due to the empirical atomic potential used.[5,22] The most accurate approach to calculate GPFE is from *ab initio* calculations, such as DFT,[23] which captures the interaction of electrons in condensed matter. Figure 3 is a GPFE curve calculated by Siegel using the DFT,[23] which will be the basis for the following discussions. We shall compare two GPFE curves calculated by the Ni potential of Cleri and Rosato (CR) (Refs. 5 and 24) and by DFT.[23]

As shown in Fig. 3, the ratio of the stable stacking fault energy γ_{sf} to unstable stacking fault energy γ_{usf} is $\gamma_{sf}/\gamma_{usf}=0.40$, which is much lower than that (0.55) calculated using CR potential. This means that after an extended partial is emitted, it is very difficult to generate the trailing partial.[5,16,24] In other words, a stacking fault can exist in the nc Ni despite its high stable stacking fault energy, and it is more stable than predicted by the MD simulations with CR potential.[5] This is consistent with the experimental observations of stacking faults in nc Ni,[20] and with the MD predictions.[5]

The disagreement between MD simulations and experiments arises in the observation of deformation twins in experiments but not in some MD simulations,[5] which claimed that Ni prefers extended partials instead of deformation twinning. Tadmor and Hai (Ref. 25) defined *twinning tendency* $T=\lambda_{crit}\sqrt{\gamma_{usf}/\gamma_{usf}}$ and Asaro and Suresh reduced T to $T=\sqrt{[1+2(1-\gamma_{sf}/\gamma_{usf})]\gamma_{usf}/\gamma_{utf}}$, with $T>1$ favoring deformation twinning and $T<1$ favoring full dislocations. T is 1.36 from DFT calculation, which is higher than the value of 1.21 calculated from MD simulations with CR potential.[5] This means that the nc Ni is easier to deform by twinning than predicted by MD simulations with CR potential.[5] The GPFE curve predicted by both methods gives higher tendency for twins than for dislocations, which agrees very well with the experimental observation of extensive twins in this study and in Ref. 20 It is not clear why twins have not been observed in MD simulations. This left some uncertainties on the stress level, grain boundary structure, grain sizes, etc., as reasons for the disagreement between the experimental observations (Ref. 20) and the MD simulations.[5]

Figure 2 indicates that the nc Ni sample deformed at high strain rate by SHPB tests has higher fraction of grains containing twins and lower fraction of grains containing

stacking faults than the nc Ni deformed at a quasistatic strain rate. This is because the flow stress during the SHPB tests was ~2.0 GPa, which is much higher than that (1.5 GPa) during the quasistatic tensile tests. The higher flow stress makes it easier to overcome the unstable twin fault energy barrier. In other words, when the nc Ni was deformed by the SHPB test, once a stacking fault is formed, the flow stress is so high that twins nucleated easily, converting stacking faults into twins, which increased the twin density and decreased stacking fault density. In addition, high flow stress also promotes emission of trailing partials, which further decreases stacking fault density.

As reported previously,[20,26] in addition to the GPFE curves, there are also several other factors that may affect the twinning tendency. They include nonequilibrius grain boundaries,[26] stress concentrations near a stacking fault and local grain boundaries,[20,26,27] and favorable orientations of twin partials.[20,26] Furthermore, we found that grain size also affects the twinning tendency, which is being studied further.

In summary, we have observed extensive deformation twins but very few stacking faults in a nc Ni tested by split Hopkinson pressure bar tests at a high strain rate of $\sim 2.6 \times 10^3\ s^{-1}$. These observations contradict the predictions of MD simulations.[5] The inaccuracy of the GPFE curves used in the MD simulations (Ref. 5) is partially responsible but cannot fully account for the discrepancies between our experimental observations and MD simulations. Other factors are also playing roles in the partial-mediated slips in nc metals, and need to be further investigated.

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