Applied Physics Letters

Partial-dislocation-mediated processes in nanocrystalline Ni with nonequilibrium grain boundaries

Cite as: Appl. Phys. Lett. **89**, 031922 (2006); https://doi.org/10.1063/1.2227639
Submitted: 04 April 2006 • Accepted: 14 June 2006 • Published Online: 20 July 2006

X. L. Wu and Y. T Zhu

APPLIED PHYSICS LETTERS **89**, 031922 (2006)

Partial-dislocation-mediated processes in nanocrystalline Ni with nonequilibrium grain boundaries

X. L. Wu[a)]
State Key Laboratory of Nonlinear Mechanics, Institute of Mechanics, Chinese Academy of Sciences, Beijing 100080, People's Republic of China

Y. T Zhu[b)]
Materials Science and Technology Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545

(Received 4 April 2006; accepted 14 June 2006; published online 20 July 2006)

The partial-dislocation-mediated processes have so far eluded high-resolution transmission electron microscopy studies in nanocrystalline (nc) Ni with *nonequilibrium* grain boundaries. It is revealed that the nc Ni deformed largely by twinning instead of extended partials. The underlying mechanisms including dissociated dislocations, high residual stresses, and stress concentrations near stacking faults are demonstrated and discussed.
[DOI: 10.1063/1.2227639]

The mechanical properties of nanocrystalline (nc) materials are controlled by their deformation mechanisms,[1] which include partial dislocation emission from grain boundaries (GBs),[2–10] deformation twinning,[9–20] full dislocations,[3,5,7] GB sliding,[3,11–13] and grain rotation.[11,14] Basing on generalized planar fault energy (GPFE) curves, molecular dynamics (MD) simulations predicted that nc Ni prefers to deform by extended partials, rather than twinning.[5] The two energies on the GPFE curves, the unstable stacking fault energy (SFE) γ_{usf} and the unstable twin fault energy γ_{utf}, are believed to play critical roles in the activation of extended partials and twining.[5] However, a recent study indicates that the γ_{usf} and γ_{utf} values obtained from GPFE curves vary significantly with the models used for their calculation and it is not clear if these values even qualitatively agree with the real values,[21] which so far cannot be experimentally measured. A recent experimental study[22] revealed the formation of both stacking faults and deformation twins in electrodeposited Ni, which has GBs not far from equilibrium and those used in MD simulations.

Nanomaterials often have nonequilibrium GBs with high densities of extrinsic (extra) dislocations.[23–25] This is especially true for those nc metals and alloys produced by severe plastic deformation.[26] It has been claimed that the GPFE curves are not applicable to these nc metals and alloys because partial dislocations already exist at/near nonequilibrium GBs and therefore do not need to be nucleated.[27,28] In other words, since the γ_{usf} and γ_{utf} only affect the nucleation process of the extended partial and the first twin partial, they should not affect the nc metals and alloys with nonequilibrium GBs. However, experimental evidence is still lacking to support such a claim.

The objective of this work is to study the partial-dislocation-mediated processes in nanomaterials with *nonequilibrium* GBs. We chose to use nc Ni produced by surface mechanical attrition treatment (SMAT) (Ref. 29) in this study because Ni has been extensively studied by MD simulations and experiments, and SMAT can produce nc Ni with impurity-free nonequilibrium GBs.

A Ni plate with a purity of 99.998% was subjected to SMAT at room temperature to produce a layer of nc Ni.[30] Extensive high-resolution electron microscopy (HREM) observations revealed that at the depth of 27 μm from the surface, the nc Ni has grain sizes in the range of 20–100 nm. The grain size is found to affect twinning propensity: twins were observed in 50% of small grains (20–50 nm) but in only 10% of large grains (50–100 nm). In contrast, stacking faults were observed in only 2% of all examined grains. These observations indicate that twinning is a more preferred deformation mechanism than slipping of extended partials.

Figure 1(a) is a HREM image showing a low angle ($\sim 3°$) GB (marked with asterisks) and a twin lamellar in a nc grain (the twin boundary is marked by an arrow). Figures 1(b) and 1(c) are Fourier filtered diffraction patterns of the low angle GB and the twin, respectively. Figure 1(d) is an enlarged image of the area inside the rectangular frame in (a). Interestingly, as indicated by the arrow on the left, a twin nucleus exists at the GB. It appears that a dissociated 60° dislocation glided toward the GB, and its wide stacking fault dynamically overlapped with the wide stacking fault of a stationary dissociated 60° dislocation on the GB, forming the twin nucleus at the GB. Such a twin nucleation mechanism has not been reported before. Shown in the right side of Fig. 1(d) is a twin with the twin boundary marked by an arrow and labeled as TB. As shown, a high density of dislocations exists on the GB segment *AB*, which is also the boundary of the twin lamellar. We believe that these dislocations were related to the twin formation process.

Figure 2 shows a nonequilibrium GB in nc Ni. Severe lattice distortion is clearly visible near the GB. Such lattice distortion attests to high residual stresses at the GB that could help with overcoming the energy barriers for nucleation of extended partials and twins.

Figure 3(a) shows a HREM image of a nonequilibrium low angle ($\sim 3°$) GB. 60° dislocations with (111) half planes are marked on the GB. Figure 3(b) is an inverse Fourier image showing much higher dislocation density on $(11\bar{1})$ planes along the same GB segment. Interestingly, Fig. 3(a)

a)Electronic mail: xlwu@imech.ac.cn
b)Electronic mail: yzhu@lanl.gov

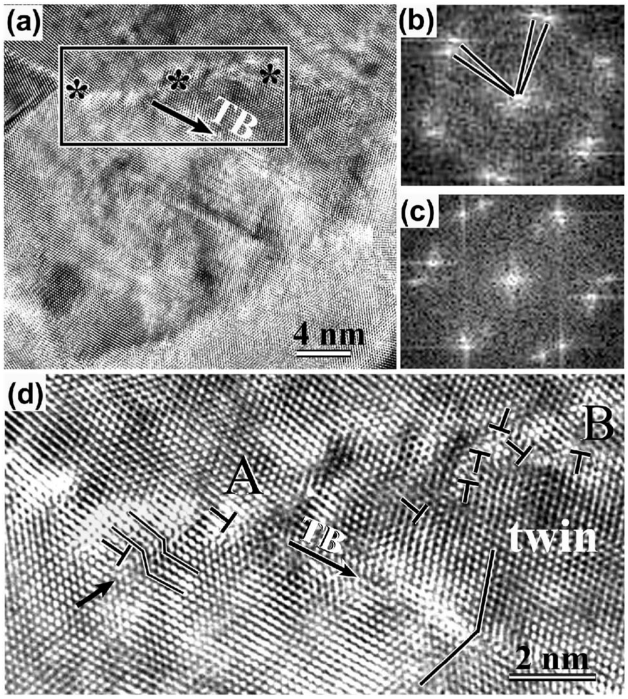

FIG. 1. (a) A HREM image showing a low angle (~3°) GB (marked with asterisks) and a twin lamellar with the twin boundary (TB) marked by an arrow. [(b) and (c)] Fourier filtered diffraction patterns of the low angle GB and twin, respectively. (d) An enlarged image of the area inside the frame in (a).

shows dissociated 60° dislocations with wide stacking faults. The boundaries of two such wide stacking faults are marked by two pairs of lines, respectively. The stacking fault widths are in the range of 6–18 atomic planes (1.22–3.66 nm). The dissociation of 60° dislocations on a GB has not been reported before and could be uniquely associated with the nonequilibrium nature of the GB.

The existence of dissociated dislocations on nonequilibrium GBs has important consequences on the deformation mechanism of nc Ni. First, the leading partial can simply slip into the grain interior under an external stress, becoming an extended partial and creating a stacking fault. In other words, the emission of the leading partial is affected by the stable stacking fault energy, but not by the much higher γ_{usf}. Second, since the trailing partials already exist on the GB, they

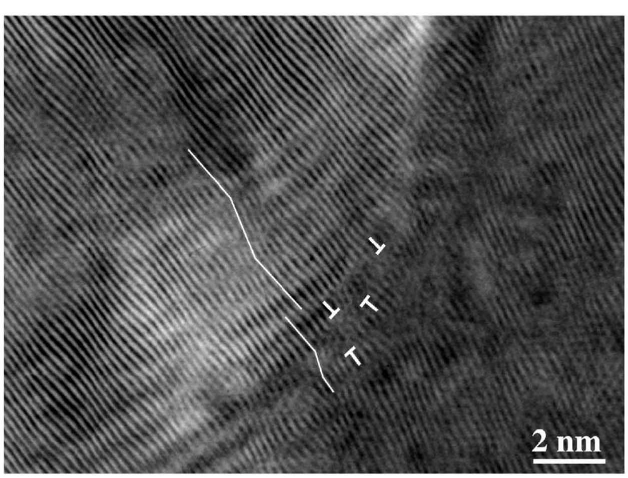

FIG. 2. A HREM image showing severe lattice distortion near a nonequilibrium GB.

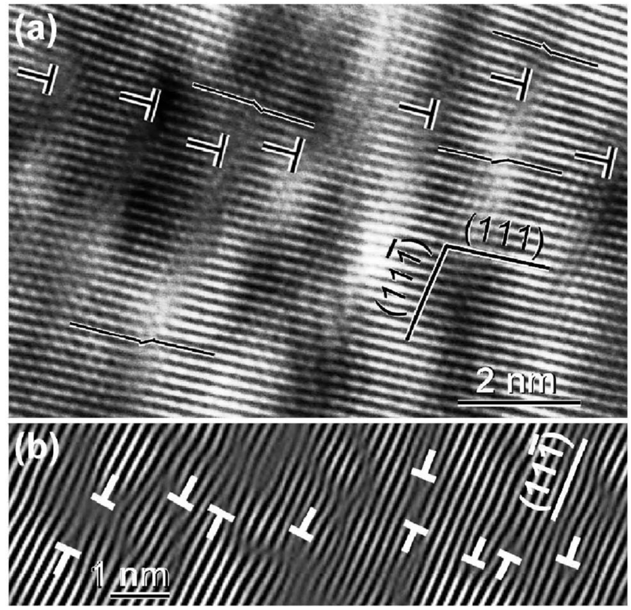

FIG. 3. HREM images showing (a) dissociation of 60° dislocations into Shockley partials bounding stacking faults on a nonequilibrium GB and (b) an inverse Fourier transformation image of high density dislocations on $(11\bar{1})$ planes. The arrow indicates the GB direction.

could also slip into the grain interior, a process that does not have to overcome the high γ_{usf}. The easy emissions of the trailing partials effectively erase the stacking faults created by the leading partial, which explains why we did not observe many stacking faults. This suggests that the γ_{usf} has no effect on the formation of stacking faults. In addition, if two dissociated dislocations on a GB happen to be on adjacent planes, a twin nucleus will form if their leading partials have the same Burgers vectors. Such a twin nucleation process will not need to overcome high γ_{utf}.

The observation of large quantities of deformation twins indicates that twins can be easily nucleated. This result is consistent with our previous reports that once a stacking fault is formed, it is relatively easy to nucleate the twin.[22] After a stacking fault is formed, a twin partial with the same Burgers vector as the initial leading partial could be emitted on an adjacent plane to nucleate a twin. Alternatively, a trailing partial could be emitted on the same plane to erase the stacking fault. An analytical model[27,28] predicts that below a certain critical grain size, it is easier to nucleate a twin partial than to emit a trailing partial. The model does not consider the γ_{usf} and γ_{utf}, and is especially applicable to nc Ni with nonequilibrium GBs studied here. The model predicted that the twinning is easiest for nc Ni with grain sizes in the range of 19–27 nm, which explains our observations that small Ni grains (20–50 nm) have a much higher twin density than larger Ni grains (50–100 nm). In addition, there are also other factors that help with the twin nucleation, including high stress concentrations near the stacking faults.[22,31]

In summary, we experimentally studied the partial-dislocation-mediated processes in a nc Ni with nonequilibrium GBs. We observed a large number of deformation twins, but very few stacking faults, contradicting the predictions by MD simulations. These discrepancies between our experimental observations and MD simulations can be explained by the following reasons. First, there are lattice distortions near nonequilibrium GBs, and the related stress concentrations are so high that they could overcome any energy barriers for nucleating partial dislocations and twins. Second, on some GBs, dislocations are already dissociated into leading and trailing partials, making the γ_{usf} irrelevant. Third, high stress concentrations near the stacking faults could help with overcoming the γ_{utf}. Fourth, we have observed a twin nucleation mechanism, dynamic overlapping of a slipping dissociated 60° dislocation with a stationary dissociated 60° dislocation on a GB. Such a mechanism is not affected by the γ_{utf}. Fifth, the GPFE curves used by the MD simulations might be significantly different from the real physical curves. Finally, a previous analytical model,[27,28] which considers the stable stacking fault energy, is applicable to nanomaterials with nonequilibrium GBs.

One of the authors (X.W.) was supported by National Natural Science Foundation of China Contract Nos. 50471086, 50571110, and 10472117 and by the National Basic Research Program of China Contract No. 2004CB619305. The other author (Y.T.Z.) was supported by U.S. DOE IPP Program Office.

[1] Y. T. Zhu and T. G. Langdon, JOM **56**, 58 (2004).
[2] V. Yamakov, D. Wolf, S. R. Phillpot, A. K. Mukherjee, and H. Gleiter, Nat. Mater. **1**, 43 (2002).
[3] D. Wolf, V. Yamakov, S. R. Phillpot, A. K. Mukherjee, and H. Gleiter, Acta Mater. **53**, 1 (2005).
[4] H. Van Swygenhoven, Science **296**, 66 (2002).
[5] H. Van Swygenhoven, P. M. Derlet, and A. G. Frøseth, Nat. Mater. **3**, 399 (2004).
[6] M. W. Chen, E. Ma, K. J. Hemker, H. W. Sheng, Y. M. Wang, and X. M. Cheng, Science **300**, 1275 (2003).
[7] X. Z. Liao, F. Zhou, E. J. Lavernia, S. G. Srinivasan, M. I. Baskes, D. W. He, and Y. T. Zhu, Appl. Phys. Lett. **83**, 632 (2003).
[8] X. Z. Liao, S. G. Srinivasan, Y. H. Zhao, M. I. Baskes, D. W. He, Y. T. Zhu, F. Zhou, E. J. Lavernia, and H. F. Xu, Appl. Phys. Lett. **84**, 3564 (2004).
[9] X. Z. Liao, Y. H. Zhao, S. G. Srinivasan, Y. T. Zhu, R. Z. Valiev, and D. V. Gunderov, Appl. Phys. Lett. **84**, 592 (2004).
[10] J. Schiøtz, F. D. Ditolla, and K. W. Jacobsen, Nature (London) **391**, 561 (1998).
[11] Z. Shan, E. A. Stach, J. M. K. Wiezorek, J. A. Knapp, D. M. Follstaedt, and S. X. Mao, Science **305**, 654 (2004).
[12] H. Van Swygenhoven, P. M. Derlet, and A. Hasnaoui, Phys. Rev. B **66**, 024101 (2002).
[13] K. S. Kumar, S. Suresh, M. F. Chisholm, J. A. Horton, and P. Wang, Acta Mater. **51**, 387 (2003).
[14] X. Z. Liao, R. Z. Valiev, H. S. Gao, X. D. Li, A. K. Mukherjee, J. F. Bingert, and Y. T. Zhu, Appl. Phys. Lett. **88**, 021909 (2006).
[15] R. J. Asaro and S. Suresh, Acta Mater. **53**, 3369 (2005).
[16] J. R. Rice, J. Mech. Phys. Solids **40**, 239 (1992).
[17] Y. M. Wang, A. M. Hodge, J. Biener, A. V. Hamza, D. T. Barnes, K. Liu, and T. G. Nieh, Appl. Phys. Lett. **86**, 101915 (2005).
[18] X. Wu and E. Ma, Appl. Phys. Lett. **88**, 061905 (2006).
[19] X. Wu, Y. T. Zhu, M. W. Chen, and E. Ma, Scr. Mater. **54**, 1685 (2006).
[20] E. B. Tadmor and S. A. Hai, J. Mech. Phys. Solids **51**, 765 (2003).
[21] J. A. Zimmerman, H. J. Gao, and F. F. Abraham, Modell. Simul. Mater. Sci. Eng. **8**, 103 (2000).
[22] X. Wu, Y. T. Zhu, and E. Ma, Appl. Phys. Lett. **88**, 121905 (2006); X. Wu and E. Ma, *ibid.* **88**, 231911 (2006).
[23] J. Huang, Y. T. Zhu, H. Jiang, and T. C. Lowe, Acta Mater. **49**, 1497 (2001).
[24] Z. Horita, D. J. Smith, M. Nemoto, R. Z. Valiev, and T. G. Langdon, J. Mater. Res. **13**, 446 (1998).
[25] X. Z. Liao, J. Y. Huang, Y. T. Zhu, F. Zhou, and E. J. Lavernia, Philos. Mag. **83**, 3065 (2003).
[26] R. Z. Valiev, Y. Estrin, Z. Horita, T. G. Langdon, M. J. Zehetbauer, and Y. T. Zhu, JOM **58**, 33 (2006).
[27] Y. T. Zhu, X. Z. Liao, Y. H. Zhao, S. G. Srinivasan, F. Zhou, and E. J. Lavernia, Appl. Phys. Lett. **85**, 5049 (2004).
[28] Y. T. Zhu, X. Z. Liao, S. G. Srinivasan, and E. J. Lavernia, J. Appl. Phys. **98**, 034319 (2005).
[29] K. Lu and J. Lu, J. Mater. Sci. Technol. **15**, 193 (1999).
[30] X. Wu, E. Ma, Y. T. Zhu, and K. Lu, in *Ultrafine Grained Materials IV*, edited by Y. T. Zhu, T. G. Langdon, Z. Horita, M. J. Zehetbauer, S. L. Semiatin, and T. C. Lowe (TMS, Warrendale, PA, 2006), p. 35.
[31] J. Wang and H. Huang, Appl. Phys. Lett. **85**, 5983 (2004).