3.22 Mechanical Properties of Materials
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Defect Nucleation in Crystalline Metals

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Please see Fig. 9a,b,c in [1].

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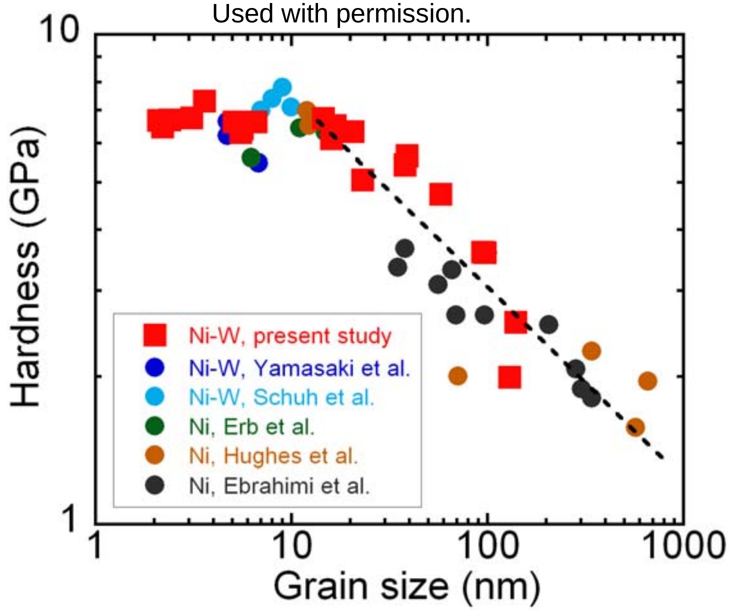
[1] Van Vliet, Krystyn J., et al. “Quantifying the early stages of plasticity through nanoscale experiments and simulations.” *Physical Review B* 67 (2003): 104105.

Big Picture

- Defect nucleation plays an important role in defect-free material volumes or if system size is reduced to the submicron level
- The stress required to nucleate a dislocation homogeneously sets an upper bound for the effectiveness of our strengthening mechanisms
- Understanding defect nucleation is part of the puzzle for understanding the breakdown of Hall-Petch scaling in nanocrystalline materials



Hardness as a function of grain size. [2]

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Defect nucleation from grain boundaries. [3]

[2] Detor and Schuh. “Tailoring and patterning the grain size of nanocrystalline alloys.” *Acta Materialia* 55 (2007): 371-379.
[3] Van Swygenhoven, H., P. M. Derlet, and A. G. Frøseth. “Stacking fault energies and slip in nanocrystalline metals.” *Nature Materials* 3 (June 2004): 399-403.

Microscopic mechanism

• When a bond breaks in shear, a new bond will usually form immediately afterwards between the new atomic neighbors. This process of bond breaking and reformation controls defect nucleation.

• The stress needed to cause such an event should correspond to the theoretical shear strength we calculated in class.

• A defect should nucleate when this stress is reached to relieve the high strain energy built up at this point

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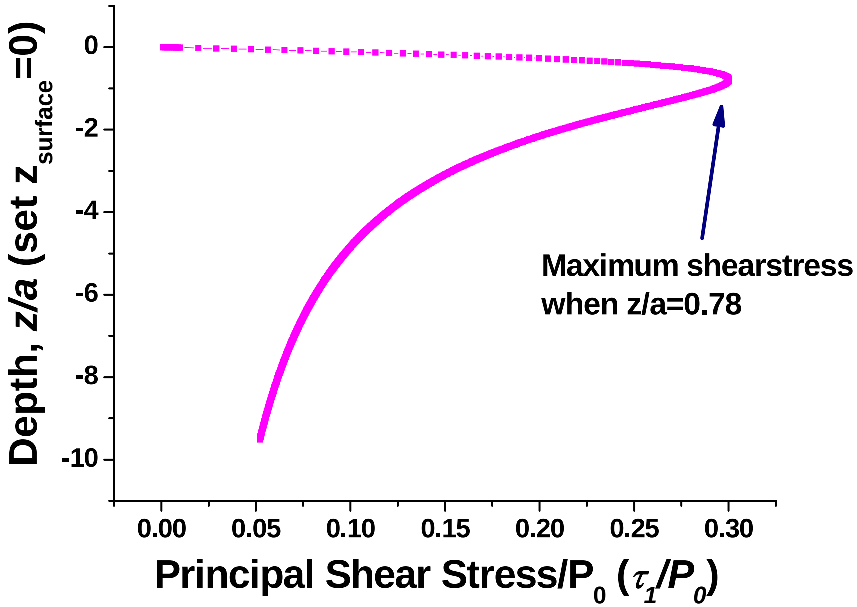
Please see Fig. 3 in [4].

In-situ TEM micrographs from [4], illustrating the response of an Al grain to nanoindentation.

[4] Minor, A. M., et al. "Direct observations of incipient plasticity during nanoindentation of Al." *Journal of Materials Research* 19 (January 2004): 176-182.

Prediction & Optimization

Defect nucleation should occur when our shear stress is maximum and near the theoretical shear stress.



Shear stress plot along the depth of the indented material by using 2D indentation model. [5]

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Please see Fig. 2 in [6].

Nucleation of dislocation at z=0.78a in bubble raft model. [6]

2D material analogs (bubble raft models), molecular dynamics simulations, and in-situ TEM indentation all support the predicted result.

[5] Johnson, K. L. *Contact Mechanics.* Cambridge, UK: Cambridge University Press, 1985.

[6] Van Vliet, Krystyn J., et al. "Quantifying the early stages of plasticity through nanoscale experiments and simulations." Physical Review B 67 (2003): 104105.