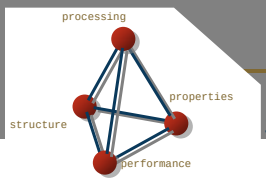
National Institute for Nano Engineering

Nanocrystalline bulk and thin film materials: Experiment and Modeling

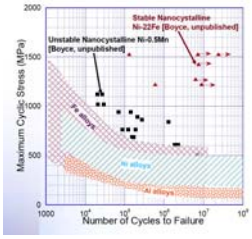
Elizabeth A. Holm
Dept. 1814



Sandia has developed a suite of experimental and computational capabilities for understanding the processing, structure, properties and performance of nanocrystalline materials.

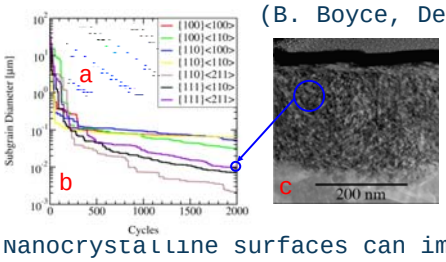
Properties and Performance

Mechanical properties



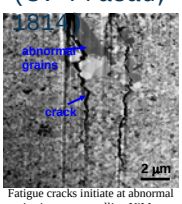
Nanocrystalline materials can exhibit exceptional mechanical properties. For example, particle-stabilized nanocrystalline nickel alloys attain cyclic fatigue lifetimes 3000 times longer than conventional nickel alloys.
(B. Boyce, Dept. 1824)

Deformation and wear



Nanocrystalline surfaces can improve friction coefficient and wear resistance. Here, FEA modeling of cyclic wear (a) predicts formation of a nanocrystalline surface layer (b) with a grain size in agreement with experiment (c).
(S. Prasad, Dept. 1824; C. Battaile, Dept. 1814)

Failure

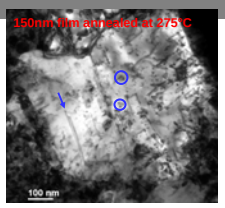


Fatigue cracks initiate at abnormal grains in nanocrystalline NiMn.

The abnormal grains that often occur in nanocrystalline metals may initiate fatigue cracks (left). Grain-scale simulations show that abnormal grains may nucleate and grow, even in a particle field, if the initial grain size is very small (right).
(B. Boyce, Dept. 1824; E. Holm, Dept. 1814)

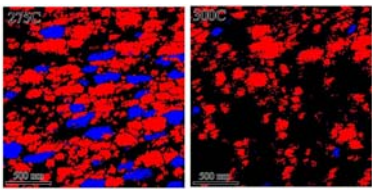
Structure

TEM



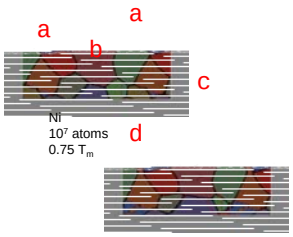
TEM reveals nanometer-scale structures in nanocrystalline materials. Here, an abnormal grain in a Ni nanocrystal incorporates twins and stacking fault tetrahedra (indicated in blue).
(D. Follstaedt, Dept. 1111)

SEM and EBSD



SEM and EBSD characterize grain structure and phase distribution. Here, large fcc (red) and hcp grains (blue) evolve differently at two annealing temperatures.
(L. Brewer, Dept. 1814)

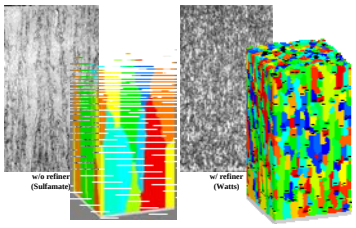
Atomic scale simulation



Atomic scale simulations capture the structure and evolution of nanoscale features. Here, large-scale molecular dynamics simulations of nanocrystalline nickel show the origin and evolution of (a)grain boundaries, (b)dislocations, (c)twins, and (d)grain topology changes.
(S. Foiles, Dept. 1814)

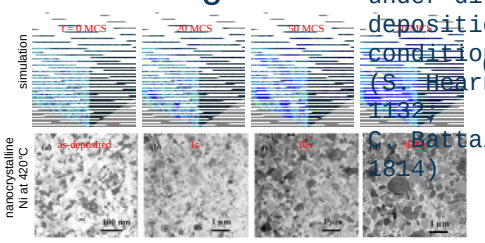
Processing

Deposition



Electrodeposition is used to form nanocrystalline metals. Here, simulations and experiments agree that the deposited structure changes from columnar (left) to equiaxed (right) under different deposition conditions.
(S. Hearne, Dept. 1132; C. Battaile, Dept. 1814)

Annealing



G. D. Hibbard *et al.*, *Scripta mater.* **47** 83 (2002).

Nanocrystalline metals evolve even at moderate temperatures. Here, simulations (a) demonstrate how the scale a nickel nanostructure changes from 25 to 500 nm upon annealing (b).
(E. Holm, Dept. 1814)

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