Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Measuring the Elastic Modulus of the Grain Boundary Component of Nanocrystalline Copper GUO-JIE GAO, YUNJIANG WANG, SHIGENOBU OGATA, Osaka University — In the past twenty years, it has been widely accepted that the Young's modulus of the grain boundary (GB) part of nanocrystalline metals is about 70% of that of the crystalline core component. However, this belief is an assumption based on numerical studies of specific grain boundary like $\Sigma 5$ twist boundary where atoms interact with one another via simplified Lennard-Jones potential at $0K$ or experimental studies assuming the GB behaves like amorphous alloys. A thorough investigation driven from completely realistic atomic simulation at finite temperature is still lacking. We reexamine this assumption by measuring the Young's modulus of pure copper (Cu) with grain size ranging from 3 to 25 nm at $300K$ using molecular dynamics (MD) uniaxial tensile tests. We implement a novel Voronoi protocol to build nanocrystalline structures of fully dense pure Cu with well-controlled grain size distribution and Mishin embedded atom model (EAM) potential. We find the following key results concerning the stiffness for nanocrystalline metals at finite temperature: 1) The GB is more thermally sensitive and therefore elastically much softer than the crystalline interior. 2) The Young's modulus of the GB is about 20% or less of that of the grain interior.

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Date submitted: 08 Nov 2012 Electronic form version 1.4