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Molecular dynamics studies of temperature and grain size effects on mechanical properties of Nanocrystalline tungsten

Abdellah Tahiri and **Idiri Boubeker**
Université Hassan II de Casablanca, Morocco

The elastic moduli of nancrystalline tungsten have been calculated from elastic constants by molecular dynamic simulation using embedded atom model. The Nanocrystal containing 16 grains with average diameters ranging from 4, 2 to 8, 9 is made using the Voronoi construction. We have been interested in the investigation of both temperature and grain size effects on elastic moduli. A softening of material was observed with the temperature increase and the grain size decrease. The anisotropy calculations have shown that the material becomes more isotropic in high temperature. The found results are in good agreement with the literature.

e: abl.tahiri@gmail.com