Mechanical Properties of Nanocrystalline Copper

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As most ordinary solids are polycrystalline, the dependence of mechanical and other properties on the size of their grains is a question of fundamental interest for materials science. The hardness of polycrystalline metals increases with decreasing grain size, in accordance to the Hall-Petch law: their hardness is a linear function of d^{-n}, where d is the average grain size and $n > 0$. On the other hand, when the grain size reaches the nanometer range, several metals have been found to exhibit a so-called "reverse Hall-Petch effect", and become softer at smaller grain sizes. Some very recent experiments show that nanocrystalline ceramics might show the same effect.

In the present work, we present simulations that demonstrate the reverse Hall-Petch effect for a typical metal (Copper). We consider fully three-dimensional model structures, having several grains of random sizes and orientations, and employ state-of-the-art Molecular Dynamics simulations. Samples are created in an automated way using the Voronoi construction method, while the grain size is deduced from sophisticated local order analysis. The properties of the material are themodynamical average values over several different samples.

We calculate structural properties and the full elasticity tensor of the material. We used the determined elastic moduli and Voigt's formulae in order to estimate the bulk-, shear- and Young's modulus of the material. Our results compare well with experimental observations. Moreover, we verify that this material becomes softer at small grain sizes. The effect is attributed to the large concentration of grain boundary atoms at smaller grain sizes. Our analysis yields scaling relations for the elastic constants as a function of the average grain size.