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Dan | Mordehai
Department of Mechanical Engineering, Technion, danmord@tx.technion.ac.il

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SIZE-DEPENDENT MECHANICAL PROPERTIES OF CRYSTALLINE NANOPARTICLES

Dan Mordehai, Department of Mechanical Engineering, Technion, 32000 Haifa, Israel
danmord@tx.technion.ac.il

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Defect-free crystalline nanostructures reach strengths which are close to their ultimate shear strength, since their deformation is controlled by dislocation nucleation from the surfaces. In this talk we examine how the size and shape of defect-free nanoparticles affect their mechanical properties. In the first part we discuss the indentation response. Earlier experiments on Au nanoparticles showed that they become easier to indent as they are smaller [1]. With large scale Molecular Dynamics Simulations, we show how the lateral dimensions give rise to size effect in indentation through the competition between dislocation storage and depletion on free surfaces. The latter mechanism is suppressed in BCC Fe nanoparticles due to strong pinning of dislocations to the indent, leading to a size-independent response to indentation [2]. Under compression, the size effect arises from a size-dependent dislocation nucleation threshold at the nanoparticle's vertices [3]. A dislocation nucleation model is employed to study how stress at which FCC nanoparticles yield depends on material properties, such as the stacking fault energy and elastic constants. The size effect is shown to disappear in Ni_3Al intermetallic nanocubes under compression, since the stress concentration vanishes in this geometry. An analysis of the dislocation evolution in Ni_3Al nanoparticles shows that partial dislocations are nucleated at the vertices, shearing the nanoparticle with large complex stacking faults planes. This combined computational-experimental study provides us with insights on how to control dislocation-nucleation controlled deformation at the nanoscale.

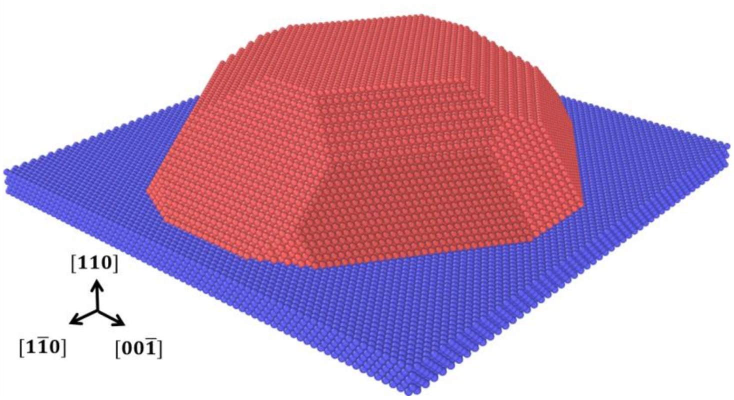

Figure 1 – A faceted Fe nanoparticle on a hard substrate in MD simulations (taken from [2]).

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