הטכניון – מכון טכנולוגי לישראל



<u>הפקולטה להנדסת מכונות</u>

<u>סמינריון</u>

הנך מוזמן/ת להרצאה סמינריונית של הפקולטה להנדסת מכונות, שתתקיים ביום הי 9.07.15 (כבי בתמוז, תשעייה), בבניין דן-קאהן, קומה 0, באודיטוריום 1 בשעה 30

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## <u>על הנושא:</u> The strength of Iron Nanoparticles

## להלן תקציר ההרצאה:

With the advancement of nanotechnology and the growing use of micro- and nano-devices, it is vital to understand the mechanical behavior of material at the small scale. In particular, it is essential to understand how mechanical properties of crystalline materials change when the sample size is reduced below one micron. At this scale, the shape and crystallographic structure plays a major role in the size-dependent strength of specimen. In this study, we examine one aspect of this problem by studying the plastic properties of iron thin-films and nanoparticles using molecular dynamics (MD) simulation. MD simulations of both indentation and compression loading are performed and the dislocation mechanisms controlling the plastic deformation are studied. In this talk we will discuss how dimensionality affects the mechanical properties of  $\alpha$ -Fe, which is the body centered cubic (BCC) lattice structure of iron, and we compare our results with previously reported studies on the deformation of face centered cubic (FCC) nanoparticles.

With indentation simulations we found that the effect of lateral facets on the indentation force is minor and that the indentation curves of thin-films and nanoparticles are similar, in contrary to what was observed in Au (FCC structure). We will show how dislocations depin themselves on different slip systems and how dislocation loops are punched into the crystal. We denote this type of deformation as "depinning controlled" and we argue that the locality of the depinning controlled deformation resulting in the lack of size-effect in indentation.

When compressing the nanoparticles along the [110] direction, dislocation are nucleated at the vertices at stress levels in the GPa regime. In this orientation, 1/2<111>{110} dislocations are nucleated on only two possible slip planes and glide into the particle towards the substrate. As the deformation proceeds, more dislocations are nucleated at the same vertices and two independent edge dislocation pile-ups are formed. However, at a certain stress level the core of the leading dislocation in the pile-up reconstructs, resulting in a stress drop and enabling further deformation. We discuss this novel reconstruction mechanism and how it is affected by the size of the nanoparticle. Finally, the simulation results are compared to some preliminary experimental results.

בברכה,

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