סמינריון

הנך מוזמן/ת להרצאה סמינריונית של הפקולטה להנדסת מכונות, שתתקיים ביום ה' 12.02.15 (כג' בשבט, תשע"ה), באודיטוריום 1 בבניין דן-קאהן, קומה 0, בשעה 14:30.

יצרה: קורן שרייבר

מנחה: פרופ"מ דן מרדכי

על הנושא:

Modeling the Strength of Ni_3Al Nanocubes Using Molecular Dynamics Simulations

להלן תקציר ההרצאה:

Materials can drastically change mechanical properties when their size is reduced to the nanoscale, mainly because of an increase in the surface to volume ratio and of lowering the amount of dislocations, which are line defects in the lattice structure. In recent years, there is a growing interest in employing mobile-dislocations free nano-particles as specimens to study strength at the nano-scale. These specimens yield at very high stresses, an indication that plasticity commences by dislocation nucleation. This observation provides us with a unique opportunity to study dislocation surface nucleation and how it is affected by the size of the nanoparticle. However, in experiments, we can only measure macroscopic properties and cannot identify mechanisms during the deformation.

In this work, we perform a molecular dynamics (MD) simulation study, to obtain insights on dislocation mechanisms which dominate the deformation of Ni_3Al nanocubes. In conjunction with experimental results that exist in literature, we provide a detailed description on how these nanocubes deform under compression. In order to interpret our results, a method was developed to identify and visualize defects in alloys. This method is parameterized in order to identify the defects in Ni_3Al, $L1_2$ crystal structure. The nanocubes deform elastically and reach compressive stress of about 7 GPa before yielding abruptly. The yield by nucleating Shockley partial dislocations at the vertices on {111} planes, leaving a symmetric structure of complex stacking faults. The mechanical response was found to be size independent, which we attribute to the cubical shape of the nanoparticle and the lack of stress gradients at its vertices. The result will be discussed in a broader context of dislocation-nucleation controlled plasticity at the nanoscale.

בברכה,

שרון אמיר

מרכז הסמינרים