הטכניון מכון טכנולוגי לישראל
TECHNION Israel Institute of Technology

הפקולטה להנדסת מכונות
Faculty of Mechanical Engineering

סמינריון

הנך מוזמן/ת להרצאה סמינריונית של הפקולטה להנדסת מכונות, שתתקיים ביום ה' 28.01.21
(ט"ו בשבט תשפ"א), בשעה 13:30 באמצעות הזום:

https://technion.zoom.us/j/96049779134

מרצה: סתו ניסני
מנחה: פרופ'/ח דן מרדכי

על הנושא:

A Multiple Site-Type Nucleation Model and its Application to the Probabilistic Strength of Pd Nanowires

The seminar will be given in Hebrew

תקציר ההרצאה:

Pristine specimens yield plastically under high loads by nucleating dislocations. Since dislocation nucleation is a thermally activated process, the so-called nucleation-controlled plasticity is probabilistic rather than deterministic like in bulk specimens, leading to a temperature-dependent distribution of the yield strength that depends on the activation parameters to nucleate dislocations. Therefore, it is essential to know the nucleation activation parameters in order to quantify the probabilistic strength at the nanoscale. Previous works showed that nucleation in nanoscale specimens, like nanowires and nanoparticles, starts from sites on the surface of the specimens, and models to relate the strength distribution to the nucleation activation parameters have been proposed. However, all models assume that all nucleation sites have the same activation parameters, which is not the case in realistic scenario. In this work, we develop a model to predict the strength distribution in nucleation-controlled plasticity when there are multiple nucleation site-types. We then apply the model to molecular dynamics (MD) simulations of Pd nanowires under tension. We found that in Pd nanowires with a rhombic cross-section, nucleation starts from the edges, either with the acute or the obtuse cross-section angles, with a probability that is temperature dependent. We show that the distribution of the nucleation strain is approximately normal for tensile at a constant strain rate. We apply the proposed model and extract the activation parameters for nucleation from both site-types. With additional nudged elastic bands simulations, we propose that the activation entropy in this case has a negligible contribution. Additionally, the free-energy barriers obey a power-law with strain, with different exponents, which corresponds to the non-linear elastic deformation of the nanowires. This multiple site-type nucleation model is not subjected only to two site-types and can be extended to more complex scenario like specimen with rough surfaces which has a distribution of nucleation sites with different conditions to nucleate dislocations.

בברכה,

פרופ"ח מתי' סאס
מרכז הסמינרים