Technion-Israel Institute of Technology
Faculty of Mechanical Engineering

הטכניון-מכון טכנולוגי לישראל
הפקולטה להנדסת מכונות

סמינריון

הנך מוזמן/ת להרצאה סמינריונית של הפקולטה להנדסת מכונות, שתתקיים ביום ה' 15.03.2018 (כ"ח באדר, תשע"ח), בניין דן קאהן, אודיטוריום 1, 13:30.

מרצה: ירדן פינטו

מנחה: פרופ'/ח דן מרדכי

על הנושא:

A Size-dependent Coupled Longitudinal-Transverse Vibration of Nanowires in Molecular Dynamics Simulations

The seminar will be given in Hebrew

תקציר ההרצאה :

In recent years, there has been a growing use of nanowires as basic building blocks for specimens and devices, such as nano-electro-mechanical systems (NEMS), nano-trusses and flexible electronics. In particular, nanowires are envisioned in nano-resonators, since their small dimensions will allow high force sensitivity, low mass and high Eigen frequency spectra. Therefore, it is desirable to study the dynamic mechanical properties of nanowires. Owing to the small surface-to-volume ratio and the internal microstructure of nanowires, they may behave differently than their bulk counterparts. Therefore, in this research we study the vibration of nanowires using Molecular Dynamics (MD) simulations, in order to obtain an atomistic-based continuum model. We focus on two types of Au nanowires, a fivefold twined nanowire (FTNW) and a single crystalline nanowire (SCNW). The former is a polycrystalline nanowire, with a pentagonal cross-section, whereas the latter has a parallelogram cross-section.

Nanowires in a cantilever configuration, with their main axis in the <110> direction, were constructed in the MD simulations, with an initial tensile strain/deflection. After relaxation, the atoms were allowed to evolve in time in the microcanonical ensemble. Several atoms on the main axis were tracked, from which the natural longitudinal and transverse frequencies of the nanowire were calculated. Comparing the results with continuum theories, we concluded that size- and shape-dependent elastic constants are required, which are extracted from the MD simulations. Based on the MD-informed continuum model we identified the slenderness ratio for which the Euler-Bernoulli predicts well the natural frequency (up to the sixth mode) and for which the Timoshenko beam model is required. Interestingly, we noticed that in some cases a longitudinal vibration of nanowires transformed into a transverse motion and vice-versa. We show that the coupling is a geometrical phenomenon that depends on the slenderness ratios of the nanowires, i.e. it occurs for ratios in the range of ~68-95 and above ~117. In the former range, the main transverse mode of deflection is the third one, whereas in the latter, the first and the fifth transverse modes prevail. We explore this phenomenon in detail and propose that higher order contributions, due to beam nonlinearities, should be considered in the continuum theory to rationalize the coupling.

בברכה,

פרופ"א מתי סאס
מרכז הסמינרים