

## סמינריון

הנדך מוזמן/ת להרצאה סמינריונית של הפקולטה להנדסת מכונות שתתקיים ביום ה' 23.01.2020  
(כ"ו בטבת, תש"פ), בניין דן קאהן, אודיטוריום 1, 13:45.

**מרצה:** תומר גור אפטר

**מנחה:** פרופ' ח דן מרדכי

**על הנושא:**

### **Using Varying Driving-Force Method to Study Activation Parameters for Nucleation – Application to the Ising Model and nucleation in nanowires**

The seminar will be given in Hebrew

**תקציר ההרצאה:**

Nucleation is a thermally activated process that appears in many processes in nature, through which the system self-assembles into a new state. One of the nucleation processes that is essential in nanomechanics is dislocation nucleation, through which dislocations - line defects that are the main carriers of plastic deformation - are formed. The nucleation is a probabilistic thermally activated process, dependent of a free energy barrier, characterized by several parameters such as the activation energy, volume and entropy. Therefore, it is imperative to calculate these activation parameters in order to quantify the strength at the nanoscale.

Recently, a varying driving-force (VDF) method was proposed in our group, to study the nucleation of dislocations. In this study, we first examine the method and validate it on nucleation of droplets in a 2D Ising model system, for which there is a closed-form solution for the activation parameters. Using the proposed VDF method, we apply an external varying field and calculate the nucleation threshold using Monte-Carlo (MC) simulations. Then, we generate a distribution of the critical external field for nucleation, and link the distribution width to the sensitivity of the energy barrier to changes in the external field, hence to the activation volume. We show that the numerically calculated activation volume is in excellent agreement with the analytically derived expression, which is strongly linked to the critical nucleus size for nucleation. At the second step, we extend the model for nucleation from multiple sites, in order to understand the effect of inhomogeneity on the nucleation process. We extend the VDF method to study the case of nucleation in a system with two different nucleation sites (with different activation parameters). This scenario was found in systems like metallic nanowires under tension and we show that the VDF model for multiple sites predicts accurately the distribution scatter of strengths, in comparison to MC simulations of the strength of nanowires.

בברכה,

פרופ' ח דן מרדכי  
מרכז הסמינרים