MECHANICAL ENGINEERING MSc SEMINAR (30 min.)

Thursday, September 18 2025 at 13:30-14:00, Zoom Meeting

Using Varying Driving-Force Method to Calculate Activation Parameters for Nucleation

Tomer Gur Apter

Supervisor: Prof. Dan Mordehai

Nucleation is a process that appears in many processes in nature, through which the system self-assembles into a new state. It is a probabilistic thermally activated process, dependent on 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. The main goal of this study is to calculate activation parameters using a varying driving force (VDF). 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.

https://technion.zoom.us/j/95159050391

Note: the seminar will be given in Hebrew

Seminars Coordinator: Prof. Dan Mordehai.