

סמינריון

הנדך מוזמנת/ת להרצאה סמינריונית של הפקולטה להנדסת מכונות, שתתקיים ביום ד'
14.02.2018 (כטי בשבט, תשע"ח), בניין דן קאהן, אודיטוריום 1, 13:30.

מרצה: בר דנינו

מנחה: פרופ' ח דן מרדכי
מנחה שותף: פרופ' דורון שילה

על הנושא:

Relations Between Material Properties and Barriers for Twin Wall Motion in Ferroic Materials

The seminar will be given in Hebrew

להלן תקציר ההרצאה:

Ferroic materials, including ferroelectrics, ferromagnetics, ferroelastic minerals, and shape memory alloys, typically exhibit a micro/nano-structure that contains twins or domains separated by twin walls. The motion of twin walls produces large deformation and governs the mechanical, electrical, and physical properties of these materials. The lattice barrier for twin wall motion is an important property that determines all the aforementioned properties. Despite that, numerical and experimental evaluations of the lattice barrier are scarce and are limited to specific materials.

The Landau-Ginzburg (LG) model is a widely accepted phenomenological phase-field model used to describe the material properties of the twin walls. However, the LG model is incapable of describing energy barriers for motion due to the lack of atomistic description. In this work, we present a general methodology for studying the relations between the lattice barrier for twin wall motion and material properties of the twin wall, which are easier to measure or calculate. An atomic model system is constructed, with a single twin wall separating crystals of different orientations. We propose a new interatomic potential and parameterize it to meet with the lattice structure of the model system and the twin wall width. After validating that the atomistic simulations are in accordance with the predictions of the LG model, a minimum energy path technique (the Nudged Elastic Band method) is employed to calculate the energy barriers for twin wall motion as a function of the wall width and the applied shear strain. The energy barrier functions extend the LG model and allow treating the motion of twin walls as a thermally activated process.

בברכה,

פז'ל'מ' איתי סאס
מרכז הסמינרים