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Topics in Modeling of Energy Systems, Mechanics of Nanomaterials, and Imperfections in Crystalline Solids

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Abstract

In 1959, physicist Richard Feynman gave a historical lecture: `*There's Plenty of Room at the Bottom'*. Even after many years, the exciting field of nanotechnology is exploding in many different directions. This talk will address some burning topics. During past few decades, the demand for energy storage has mushroomed both for portable and static applications. Hence we considered two types of problems in energy systems: atomistic mechanism of phase boundary formation during initial lithiation in crystalline silicon and 2D materials for energy storage. We discovered that defective graphene would be a potential anode material for different ion batteries because of the underlying charge-transfer mechanism governing the enhanced adsorption of adatoms. Besides energy systems, graphene can be used in heterostructures, nanocomposite, and healthcare. But if nanomaterials such as graphene are used in real-life applications, mixed-mode fracture is inevitable because of the externally applied complex loading. Therefore, we studied graphene with crack like flaw and investigated the complex mixed-mode fracture behavior. However for practical industry applications, crystalline solids are mainly used instead of nanomaterials. Imperfections such as dislocations are inherently present in these solids. We developed models for the dislocation pattern formation resulting in grain boundary structures. Phase-field modeling is another approach for modeling grain boundary evolution. We developed new multi phase-field model for dynamic recrystallization taking into account crystal orientations and many practical situations. However, for major real-life applications, alloys are used instead of perfect crystals. Since we don't know *a priori* many materials properties of these alloys, indentation experiments are very much essential. We developed methods that can take experimental indentation data as input and determine necessary materials parameters. All these findings will provide useful guidelines for the design of energy systems, nanodevices, and various practical applications.

Bio

Dr. Dibakar Datta is currently a postdoctoral research scholar in Mechanics and Computation group at Stanford University. He received his PhD from Brown University in 2015 with major in Solid Mechanics and minors in Physics and Chemistry. While at Brown, he was a visiting scholar in the Department of Materials Sciences and Engineering at the University of Pennsylvania for a year. Before moving to United States, he completed his studies in India, Spain, and France. His research focuses on the modeling of energy systems, atomistic mechanics of nanomaterials, and modeling imperfections in crystalline solids.