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Nanomechanics Simulation Toolkit – Dislocations Make or Break Materials

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ABSTRACT

The goal of computational material science is to improve existing materials and design new ones through mathematical calculations. In particular, molecular dynamic simulations can allow for visualization of dislocations in a material, along with its resulting behavior when under stress. For example, plastic deformation and strain hardening result from the movement, multiplication and interaction of dislocations within the crystal structure. A simulation tool to study these phenomena was developed for the nanoHUB web resource as a part of the Network for Computational Nanotechnology at Purdue University and targets audiences ranging from undergraduate students to researchers. We created a user-friendly environment to explain the complicated nature of dislocations on a basic level for undergraduate students, while enabling researchers to modify advanced inputs. The output of the tool provides both quantitative graphs and visual animations, essential for anyone trying to understand how dislocations either move or nucleate. In its default state, the tool will access loader files that generate simulations with pre-determined inputs in order to accelerate usage. More advanced users can manipulate parameters, such as simulation run time and dislocation type, to fit their individual needs. The tool can provide a useful framework both as an instructional device in material science courses as well as a simulation framework for researchers. Furthermore, web resources like this provide understandable feedback for modeling and verifying ongoing research projects.

KEYWORDS

dislocations, Graphical User Interface, material science, nanoHUB, Cloud Computing