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Crack Propagation Simulation Tool

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ABSTRACT

In the massively engineered world that exists today, understanding material behavior is of paramount importance in caring for human safety in design. Molecular dynamic simulations on crack propagation through materials allow visualization of material behavior under stress. The tool, developed by the nanoHUB group as a part of the Network for Computational Nanotechnology at Purdue University, makes performing such simulations accessible to undergraduate students, highly qualified researchers, and all those in between. First, the input deck for the simulation parameters was simplified from the complex, language-specific code into a simple, user-friendly Graphic User Interface (GUI). Several interesting example cases were run through using the GUI and developed to help the user understand the functionality of the tool. The output of the GUI was developed to allow the user to have both numerical and visual depictions of what occurred. The resulting tool allows for a step-by-step walkthrough of generating the case in situations where the user may be unfamiliar with the required code. The user can manipulate the parameters to fit their individual needs in regards to size and strain rate for example. The tool can be used as instructional material in classes such as materials science and validation material for the varied clientele that exists. This nanoHUB tool will contribute to educating future engineers and scientists in materials behavior. Furthermore, it provides engineers and scientists a simple process to model and validate their ongoing projects and research.

KEYWORDS

Crack, Molecular Dynamics, Simulation, Graphic User Interface, Materials

REFERENCES

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