ABSTRACT

Fortuitous crack propagation rendering unexpected material failure is ubiquitous in many cases. For example, ships in World War II collapsed because of crack propagations and contemporary it can be even encountered inside the Boeing 737 fuselage. This leads to the essence of conducting research on the factors that affect the ductility of the material. An experimental study like tensile test is not fastidious enough to control the temperature and stress around crack tip and it is not able to give atomic level details such as how the crack propagates and the bonds break when the materials are subjected to the critical stress. Therefore creating a simulation tool for the crack propagation will be a better solution for the problem. The simulation tool is created in the rappture builder to interface user inputs with LAMMPS (molecular dynamic (MD) tool) code. The basic function allows the users to select the materials, strain rate, and temperature which are the key parameters affecting crack propagating. Also the tool provides more option that allows the users to modify the parameters in simulation such as the crack size, the crystal structure, the strain direction etc. It will demonstrate the user stress vs strain curve and an animation of the crack propagation. The tool will not only help people who are interested in this mechanical property of materials to learn the details about crack propagation but also to do higher level research based on my simulation tool.

KEYWORDS

Crack propagation, LAMMPS, simulation