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Mark S Korlie^{*} (korliem@mail.montclair.edu), 1 Normal Avenue, Upper Montclair, NJ 07043. *Molecular Dynamics Simulation of Cracks and Fractures in A Solid*. Preliminary report.

We use Lennard-Jones potential like formulas to derive dynamical equations for the atoms/molecules in a solid. The resulting systems of nonlinear ordinary differential equations are then used to simulate the evolution and propagation of cracks and fractures in the solid. For application, we use a 3-D sheet of ice, where the ice molecules are both stressed and compressed. Computer examples compare dynamical responses when the solid has a slot or does not have a slot. The mechanisms for both cracks and fractures development are presented and discussed. (Received October 03, 2000)