ATOMIC MECHANISM OF NEAR THRESHOLD FATIGUE CRACK GROWTH IN VACUUM AS A BASIS FOR UNDERSTANDING ENVIRONMENTAL EFFECTS

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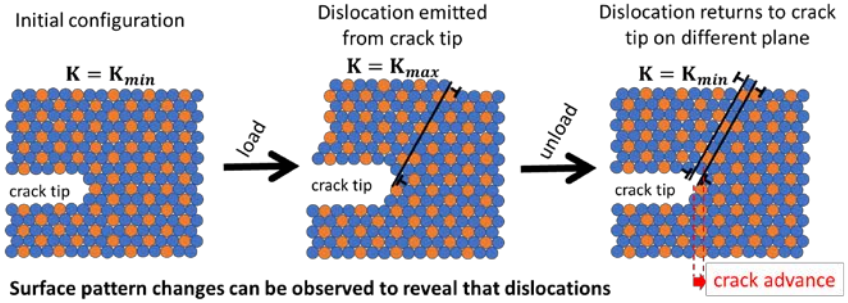
Key Words: Fracture, Molecular Dynamics, Simulation, Cleavage, Hydrogen

The growth of cracks governs engineering decisions across a broad range of industry. Yet, in many technologically relevant regimes, the process by which cracks grow remains unknown. A prime example is near-threshold fatigue crack growth in vacuum environments, which *constitutes the foundation from which environmental effects can be understood*. In this case, crack growth per loading cycle can be on the order of angstroms, inhibiting direct observation of the material separation process. Accordingly, atomistic modeling is the best available tool to better understand the phenomenon.

While a large atomistic modeling literature exists, the link between modeled cracks and laboratory behavior is complicated by disconnects in stress state, simulation geometry, and thermal activation. In cases where care has been devoted to modeling a well-developed cyclic stress field, fatigue crack growth has been reported. However, such modeling outcomes occur at loading amplitudes well below the corresponding experimentally observed thresholds for fatigue crack growth in vacuum.

The cyclic loads associated with experimentally observed fatigue crack growth thresholds entail micrometers of deformation at the crack tip. This well surpasses modern atomistic modeling capabilities, which at best could simulate a sufficient 2D domain for 10's of loading cycles (with a dedicated ExaFLOP supercomputer using ~ $500,000 of electricity). This challenge has limited the focus of previous studies towards nanometer cracks, lower loading amplitudes, and few loading cycles. A concurrent multiscale approach addresses the challenge by reducing degrees of freedom, allowing larger simulation domains to be studied over more cycles without sacrificing atomic resolution at the crack tip. For crack behavior, the multiscaling is complicated by the movement of dislocations over large distances, and thus, a coupled atomistic discrete dislocation (CADD) approach is necessary.

Here, I will report on atomistic simulations to cycle counts far beyond those analyzed previously by harnessing contemporary computational resources and a parallel implementation of the CADD concurrent multiscale approach. Our simulations show that fatigue crack growth arrests after an initial transient period, reconciling the standing discrepancy between model and experiment. With this understanding, we will then examine hypothesized mechanisms for near threshold fatigue crack growth in vacuum. Finding sustained crack growth to only occur when edge dislocations return to the crack tip on a slip plane behind the one on which they were emitted. This process transfers material away from the crack tip, supporting a long-ago hypothesized necessity for near threshold fatigue crack growth in vacuum (Cottrell, 1957; Mott, 1958). The movement of material away from the crack tip inhibits the rewelding of crack faces at the bottom of the load cycle, consistent with carefully executed laboratory observations (Laird, 1963; Vasudevan, 1995).



Surface pattern changes can be observed to reveal that dislocations changed planes during a fatigue loading cycle and produced crack growth