Molecular Dynamics Simulation of Crack Tip Processes in Alpha-Iron and Copper

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The intrinsic crack tip processes of either propagation by cleavage or blunting by the nucleation of dislocations from the non-linearly stressed region at the crack tip have been simulated by a molecular dynamics approach in alpha-iron and in copper, utilizing the Johnson and Morse potentials, respectively, and a new fixed stress boundary condition at the border between the inner discrete region and the outer anisotropic linear continuum. The simulations showed that alpha-iron is inherently brittle and fails by cleavage along a cube plane when the stress intensity factor reaches the critical Griffith value. No dislocations are nucleated in iron and even the development of restricted crack tip twinning in special orientations does not alter this intrinsic brittleness. In copper crack tip blunting at a level somewhat less than the Griffith stress intensity factor always prevented brittle crack growth by cleavage. Thus, copper is inherently ductile. Because it permitted the unhindered development of substantial nonlinear crack tip displacements, and did not prevent dislocation from penetrating through the border between the inner nonlinear material and the outer linear continuum, the new stress boundary condition was found to be far superior to the fixed or flexible boundary conditions used at this border by previous investigators. This is reflected in the observed critical stress intensity factors for brittle cleavage that were found to be nearly equal to the expected Griffith value for the stress boundary condition while the displacement boundary conditions gave results nearly three times higher.