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Ab initio prediction of environmental embrittlement at a crack tip in aluminum

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This talk reports on our *ab initio* predictions of environmental embrittlement in aluminum. We have used an atomistic-continuum multiscale framework to simulate the behavior of a loaded crack tip in the presence of oxygen and hydrogen. The multiscale simulations and subsequent analysis suggest that electronegative surface impurities can inhibit dislocation nucleation from a loaded crack tip, thus raising the likelihood for incremental brittle crack growth to occur during near-threshold fatigue. The metal-impurity bonding characteristics have been analyzed using a Bader charge transfer approximation, and the effect of this bond on the theoretical slip distribution has been investigated using a continuum Peierls model. The Peierls model, which is a function of the position dependent stacking fault energy along the slip plane, was used to estimate the effects of several common environmental impurities.