

Abstract Submitted  
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**The formation and structure of the oxide and hydroxide chemisorbed phases at the aluminum surface, and relevance to hydrogen embrittlement** MICHAEL FRANCIS, ROBERT KELLY, MATTHEW NEUROCK, University of Virginia — Aluminum alloys used in aerospace structures are susceptible to environmentally assisted cracking (EAC) induced by hydrogen embrittlement (HE) (Gangloff and Ives 1990). Crack growth experiments have demonstrated a linear relation between the relative humidity of the environment and crack growth rates, indicating the importance of water (Speidel and Hyatt 1972). While the presence of water has been demonstrated to be necessary for EAC of aluminum, crack growth rates have been linked to the diffusivity of hydrogen in aluminum (Gangloff 2003) and hydrogen densities at the crack tip as high as  $\text{Al}_2\text{H}$  have been observed (Young and Scully 1998). While the mechanism by which hydrogen embrittles aluminum is yet not well understood, without the entry of hydrogen into the aluminum matrix, embrittlement would not occur. While at the crack tip high hydrogen concentrations exist, the solubility of hydrogen in aluminum is normal near 1 ppm (Wolverton 2004). In this work combined first principles and kinetic Monte Carlo methods will be used to examine the oxide and hydroxide structure resulting from exposure of aluminum to  $\text{H}_2\text{O}$  or  $\text{O}_2$  and relevance to hydrogen entry as well as EAC is discussed.

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