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Aluminum/water reactions under extreme conditions

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We discuss mechanisms that may control the reaction of aluminum and water under extreme conditions. We are particularly interested in the high-temperature, high-strain regime where the native oxide layer is destroyed and fresh aluminum is initially in direct contact with liquid or supercritical water. Disparate experimental data over the years have suggested rapid oxidation of aluminum is possible in such situations, but no coherent picture has emerged as to the basic oxidation mechanism or the physical processes that govern the extent of reaction. We present theoretical and computational analysis of traditional metal/water reaction mechanisms that treat diffusion through a dynamic oxide layer or reaction limited by surface kinetics. Diffusion through a fresh solid oxide layer is shown to be far too slow to have any effect on the millisecond timescale (even at high temperatures). Quantum molecular dynamics simulations of liquid Al and water surface reactions show rapid water decomposition at the interface, catalyzed by adjacent water molecules in a Grotthus-like relay mechanism. The surface reaction barriers are far too low for this to be rate-limiting in any way. With these straightforward mechanisms ruled out, we investigate two more complex possibilities for the rate-limiting factor; first, we explore the possibility that newly formed oxide remains a metastable liquid well below its freezing point, allowing for diffusion-limited reactions through the oxide shell but on a much faster timescale. The extent of reaction would then be controlled by the solidification kinetics of alumina. Second, we discuss preliminary analysis on surface erosion and turbulent mixing, which may play a prominent role during hypervelocity penetration of solid aluminum projectiles into water.