

Ab Initio Mechanical Properties of Alumina Polymorphs for Cold Spray Al Powder Passivation Layers

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Cold spray of aluminum powders is heavily influenced by the passivation layer which natively forms under ambient conditions. Under humid atmospheric conditions at room temperature, this passivation layer can readily thicken, resulting in an increased critical adhesion velocity and thus reduced bonding and deposition efficiency. For structural repair applications, bonding is of critical importance; however, it is unclear whether passivation layer crystallinity, thickness, and composition or some combination thereof is principally responsible for this increase. Furthermore, experimental characterization of the several nanometer thin passivation layers is incredibly difficult. Though extensive computational work has been performed on alumina and its various dry and hydrated polymorphs these are often restricted by empirical force fields, isolated systems or varying simulation parameters that inhibit direct comparisons. Here, we investigate the mechanical properties of crystalline and amorphous, dry and hydrated alumina polymorphs using density functional theory. Ideal strength and elastic computations are extrapolated to critical adhesion velocity through semi-empirical shock relations previously developed for single particle impact. These results give credence to thickness and crystallinity being the main drivers of increases in critical adhesion velocity.