Lithium Segregation Induced Structure and Strength Change At Amorphous-Si/Cu Interface

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Silicon anodes with excellent performance have been demonstrates utilizing nanoengineered composite structures that combine high capacity and mechanical stability with high electrical conductivity. The present paper is aimed to provide a quantitative interpretation of lithiation at the interface of Li_xSi/Cu using both atomic simulations and experimental analysis. Our results demonstrate that the lithium concentration at the a-Si/Cu interface is higher than that in the bulk, indicating lithium segregation at the a-Si/Cu interface. We then calculate both the tensile and shear strength at the Li_xSi/Cu interfaces through *ab initio* molecular dynamics (AIMD) and density functional theory (DFT), with results revealing that charge transfer from lithium to Cu and its segregation are responsible for weakened interface strengths.