Title:	A theoretical study of aluminium doping in silicon anode based lithium-ion batteries using ReaxFF molecular dynamics simulation
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Abstract:	Silicon and Aluminium are abundant elements in nature. Silicon materials have higher capacity that can be used as a replacement for the graphite anode. However, due to mechanical failure and self-degradation during battery operation, Si is not suitable to be used as an anode in LIBs. The cycle performance of LIBs depends on the diffusion of Li within anode material. The high energy barrier of the Si structure results in lesser kinetic transport of Li, hence Si anode is not feasible to be used in LIBs. In the past, many approaches were proposed to improve the rate performance of Si anode that includes doping, porosity, amorphicity, and geometry tailoring. In this paper, the ReaxFF interatomic potential and MD simulations were conducted to study the kinetic behavior of aluminium doped amorphous lithiated silicon (a-LixSiAly) compounds. The results suggest that by doping of aluminium, the coefficient of diffusion improves, although there is no relation found between the amount of dopant and diffusivity. We replaced dopant aluminium with alumina and studied the structural and kinetic behavior of silicon anode based lithium-ion batteries (LiSi). Our results show that the specific amount of alumina can improve diffusivity but is not as significant as in the case of aluminium. We used hybrid GCMC/MD simulations to compute the open-voltage profiles during the cell discharge operation. These simulation results provide an interesting relation between Li and Al content in the compound for voltage discharge profile. Doping of aluminium and its amphoteric oxide can increase the diffusion coefficient of Li in LiSi batteries. A specific amount of doping improves the battery discharge voltage profile. To the best of the authors understanding, not much research has been carried out on this idea. The present research results suggest the improved capacity and cycle performance of batteries. The voltage profile diagrams suggest an exponential relation between aluminium and lithium content while doping, and this can be used in the industrial manufacture of LiSi batteries. The Al2O3 doping results in a parabolic curve, which clarifies the specific amount of dopant that can lead to the highest performance.
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