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Li and Si diffusion in Si anodes in Li-ion batteries: An *ab-initio* molecular-dynamics-based study PRIYA JOHARI, VIVEK B. SHENOY, Division of Engineering, Brown University, Providence RI 02912, USA. — Several studies have been carried out in the past few years to understand the dynamics of Li diffusion in Si anodes of Li-ion batteries, however, most of these studies are restricted to the diffusion of a single Li atom in crystalline Si. While, it is well known that crystalline Si becomes amorphous on lithiation, this phenomenon has not been considered in previous computational work. Here, we report the results of molecular dynamics simulations that were carried out to study the diffusion of Li atoms in crystalline as well as amorphous Si for the LiSi phase. We have also analysed the dynamics of the Si atoms during lithiation to understand its role in stress generation/relaxation. We find that Li diffuses faster in amorphous Si as compared to crystalline Si, while the diffusivity of Si is around two orders of magnitude lesser than Li.

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