Lithium effects on the mechanical and electronic properties of germanium nanowires

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Semiconductor nanowire arrays promise rapid development of a new generation of lithium (Li) batteries because they can store more Li atoms than conventional crystals due to their large surface areas. During the charge-discharge process, the electrodes experience internal stresses that fatigue the material and limit the useful life of the battery. The study of the electronic properties of lithiated nanowire arrays using theoretical models allows designing electrode materials that improve battery performance. In this work, we present a density functional theory study of mechanical and electronic properties of germanium nanowires (GeNWs) grown along the [111] crystallographic direction with a diamond structure and surface passivated with hydrogen (H) and lithium (Li) atoms. The study is performed within the local density approximation. The results show that the energy gap is a function of both the Li concentration and the nanowire diameter. Furthermore, the Young's modulus (Y) increases with the nanowire diameter, in agreement with experimental reports. The increase in the Li concentration at the nanowire surface leads to a larger Y value compared to that of the completely H-passivated one, except for the thinner nanowires where the Y stays almost constant. These results demonstrate that it is possible to simultaneously control the energy gap and the Young's modulus by tuning the Li concentration on the surface of the GeNWs and they could help to understand the structural changes that GeNW arrays experience during the lithiation process in Li batteries.

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