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Studies of $Si_{1-x}O_x$ Electrode Materials Prepared by Combinatorial Sputter Deposition

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Silicon (Si) has a high theoretical capacity (3578 mAh/g. Such a high capacity has made it an active area for research in the last two decades. However, one of the main challenges with crystalline Si anode is its rapid fading capacity after only a few cycles. The main cause for such a behavior is the large volume change that takes place during the insertion and extraction of lithium. Such a huge change (280%) leads to the pulverization of the anode material. Based on previous studies, it is our opinion that silicon-based amorphous alloys are promising when used as a negative electrode. In the current work, thin films of $Si_{1-x}O_x$ were produced using combinatorial sputtering methods. The amorphous or nanostructured nature of the prepared samples was confirmed by the revealed X-ray diffraction measurements. Cyclic voltammetry method was employed to evaluate the electrochemical performance of the samples. The specific capacity as a function of oxygen content is reported. It was found that the irreversible capacity increases with oxygen content. The measured reversible specific capacity is consistent with our proposed model which assumes that $Si_{1-x}O_x$ is made up of amorphous silicon, which can react to form $Li_{3.75}Si$, and amorphous SiO_2, which in turn reacts to form Li_4SiO_4. . Also, our model is consistent with the structure of the computed Li-Si-O ternary phase diagram which suggests that lithium reacts with SiO_2 matrix to form Li_4SiO_4. Then, lithium starts to alloy with Si particles to from $Li_{15}Si_4$, the most lithiated phase at room temperature. However, $Li_{15}Si_4$ is not shown in the equilibrium phase diagram. The formation of Li_4SiO_4 may not only work as a buffer matrix that minimizes the volume expansion during the insertion of lithium but it may also enhance the diffusion of lithium into the nano silicon phase. In conclusion, the irreversible capacity in SiO_x increases with oxygen content because of the formation of Li_4SiO_4. Nevertheless, the formation of inactive Li_4SiO_4 may improve cycleability. As a result, the optimization of oxygen content is a must.

Keywords: thin films; negative electrode; silicon