

Reaction Mechanism and Performances of Pioneer 2D $\text{Si}_x\text{Ge}_{1-x}\text{H}$ Electrodes in Lithium-ion Batteries

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Abstract

2D monoelemental materials, such as silicene and germanene, have recently received a lot of attention due to their tunable structures and remarkable physicochemical properties [1,2]. The addition of covalently bonded hydrogen in the z-orientation of each silicene and germanene atom results in hybridized bonding site changes from sp^2 to sp^3 with new terms of silicane (*i.e.*, hydrogen-terminated silicene, SiH) and germanane (*i.e.*, hydrogen-terminated germanene, GeH) [3,4]. However, challenges in the synthesis of such materials impede their detailed study, exploitation, and applications. In this work, we present pioneer 2D silicane and germanane materials with different compositions, namely, $\text{Si}_{0.25}\text{Ge}_{0.75}\text{H}$, $\text{Si}_{0.5}\text{Ge}_{0.5}\text{H}$, and $\text{Si}_{0.75}\text{Ge}_{0.25}\text{H}$ that benefit from the simultaneous presence of both Si (high capacity) and Ge (high-rate performance and capacity retention). The three samples were synthesized through simple and efficient chemical exfoliation of bulk Zintl phases. The presence of both SiH and GeH in a single structure offers a synergistic beneficial effect on the electrochemical performances of $\text{Si}_x\text{Ge}_{1-x}\text{H}$ (with x values from 0.25 to 0.75). Among them, the $\text{Si}_{0.5}\text{Ge}_{0.5}\text{H}$ electrode shows the highest capacity, up to 1526 mAh g^{-1} after 20 cycles. The $\text{Si}_{0.5}\text{Ge}_{0.5}\text{H}$ electrodes were respectively, subjected to 0, 10, 100, and 200 half-cell cycles followed by *ex-situ* SEM and SEM-EDX analysis to assess the effects of lithiation/delithiation and alloying/dealloying on the $\text{Si}_{0.5}\text{Ge}_{0.5}\text{H}$ flakes. Figure 1 shows the variations in morphology after different cycles.

References

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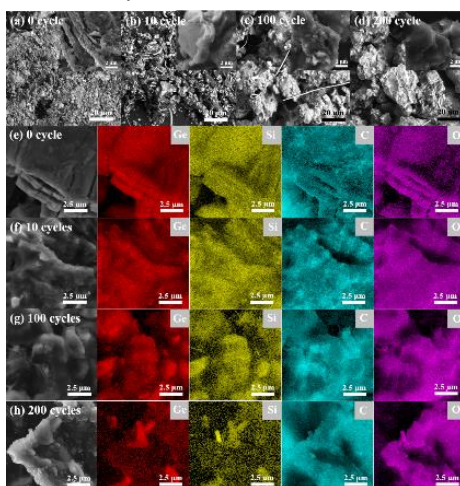


Figure 1: SEM and SEM-EDX images depicting the progression of deformation caused by lithiation and delithiation on the $\text{Si}_{0.5}\text{Ge}_{0.5}\text{H}$ morphology upon cycling.