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Sub-oxide passivation of silicon nanoparticles produced by mechanical attrition

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The presence of native oxide on the surface of silicon nanoparticles is renowned for constraining charge transport on the surfaces. Studies carried out using scanning electron microscopy (SEM) shows that the particles in the printed silicon network have a wide range of shapes and sizes. High-resolution transmission electron microscopy reveals that the particle surfaces are dominated by the (111)- and (100)-oriented planes which stabilizes against further oxidation of the particles. X-ray absorption spectroscopy (XANES) and X-ray photoelectron spectroscopy (XPS) measurements at the O 1s-edge have been utilized to study the oxidation and local atomic structure of printed layers of silicon nanoparticles which were milled for different times. XANES results reveal the presence of the +4 (SiO_2) oxidation state which tends towards the +2 (SiO) state for higher milling times. Si 2p XPS results indicate that the surfaces of the silicon nanoparticles in the printed layers are only partially oxidized and that all three sub-oxide, +1 (Si_2O), +2 (SiO) and +3 (Si_2O_3), states are present. The analysis of the change in the sub-oxide peaks of the silicon nanoparticles shows the dominance of the +4 state only for lower milling times.

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