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Integrated Computational Materials Process and Product Engineering.

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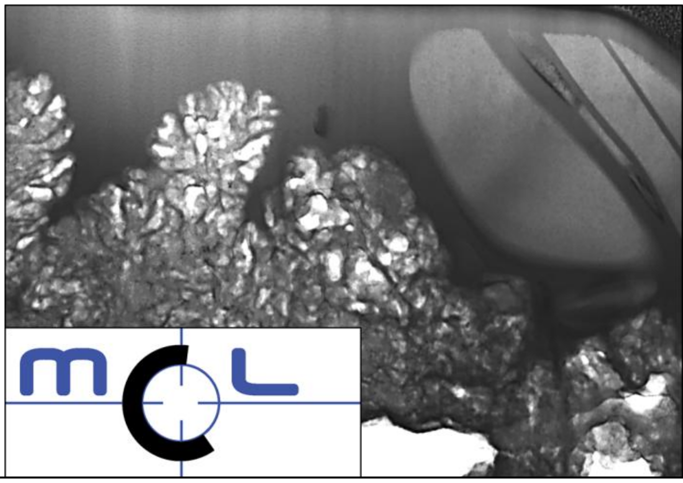

Transmission electron microscopy image of a grown amorphous silicon–electrolyte composite layer after 300 charge/discharge cycles. Image: MCL

A NEW PERSPECTIVE ON THE DEGRADATION OF SILICON-BASED ANODES

THE SIGNIFICANT VOLUME CHANGES OF SILICON DURING CHARGING AND DISCHARGING LEAD TO STRUCTURAL TRANSFORMATION (AMORPHIZATION) OF THE MATERIAL, WHICH PLAYS A DECISIVE ROLE IN DETERMINING THE CAPACITY AND LIFETIME OF LITHIUM-ION BATTERIES.

The transition to electrification requires lithium-ion batteries with higher energy density, improved cycle stability, and longer lifetimes. Achieving requires new electrode materials to drive the next generation of batteries forward. Silicon (Si), with its high energy capacity, holds enormous potential for lithium-ion batteries (LIBs) and solid-state batteries (SSBs), opening up new possibilities in energy storage.

Despite advances in understanding the electrochemical properties of Si anodes, the effects of volume changes and mechanical stresses on the crystalline structure of silicon remain insufficiently explored. It is assumed that degradation is primarily driven by the reformation of the silicon-electrolyte interphase (SEI). Cracks in the SEI layer expose fresh silicon, leading to repeated SEI growth and, consequently, the formation of a thick silicon–electrolyte composite layer (SEC). In addition to these chemical processes, lithium insertion into silicon particles also induces a transition from the crystalline to the amorphous phase.

Studies show that similar phase transitions occur under mechanical stress, such as compression or nanoindentation. In this context, shear bands and crystallographic defects destabilize the crystal lattice.

Our research, using 4D-STEM, FESEM, synchrotron X-ray nanotomography, and AI-assisted microstructural analysis, demonstrates that shear bands can form in Si-based anodes, triggered by stresses during cycling.

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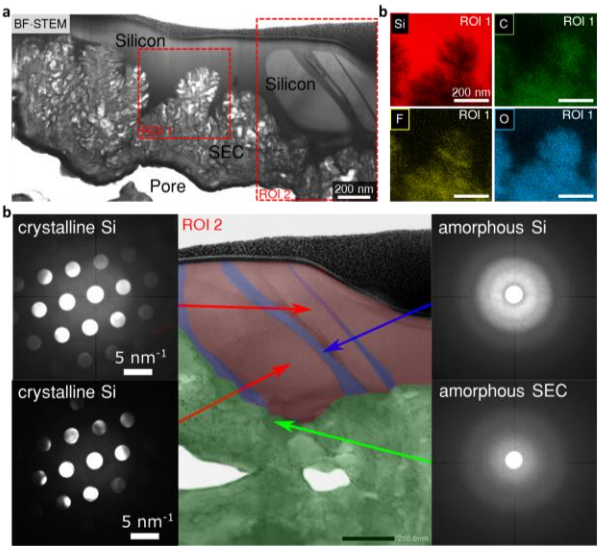
These transitions promote uneven SEC growth and alter the stress distribution within the anode. Additionally, phase-dependent lithiation rates accelerate these processes. Surprisingly, these phase transitions may have a stabilizing effect in the long term by reducing crack formation and particle fracture, thereby delaying battery failure.



On the left, the lithiation (red) evenly surrounds the silicon particle (cyan), while the complex pattern on the right (blue) accelerates battery aging.

Impacts and Outlook

This study highlights the interplay between mechanical and chemical degradation processes and provides new insights into silicon anodes. Controlling interfacial kinetics and developing optimized silicon architectures are critical for advancing energy storage technologies. In collaboration with Materials Center Leoben Forschung GmbH, Montanuniversität Leoben, the Austrian Academy of Sciences, Varta Innovation GmbH, and ESRF – The European Synchrotron, we established a foundation for future innovations in battery technology

M. Häusler et al. Amorphous shear band formation in crystalline Si-anodes governs lithiation and capacity fading in Li-ion batteries. Commun Mater 5, 163 (2024).

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