SPP 1473 - WeNDeLIB: Join-Project #12: Thermodynamics and kinetics for stabilization of conversion-type electrodes for lithium-ion batteries based on nanoscaled 3d transition metal oxides

Subproject #3: Microstructure features behind the degradation of nanocrystalline 3d transition metal oxide composites in conversion type electrodes for lithium-ion batteries

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The aim of the project #12 is to improve the bad cycling stability of the electrode materials that are based on the conversion mechanism. The aim of the subproject #12 in particular is to understand the microstructure features behind the degradation of nanocrystalline 3d transition metal oxide composites in conversion type electrodes, which is the first step to the improvement of the cycling stability of these electrode materials.

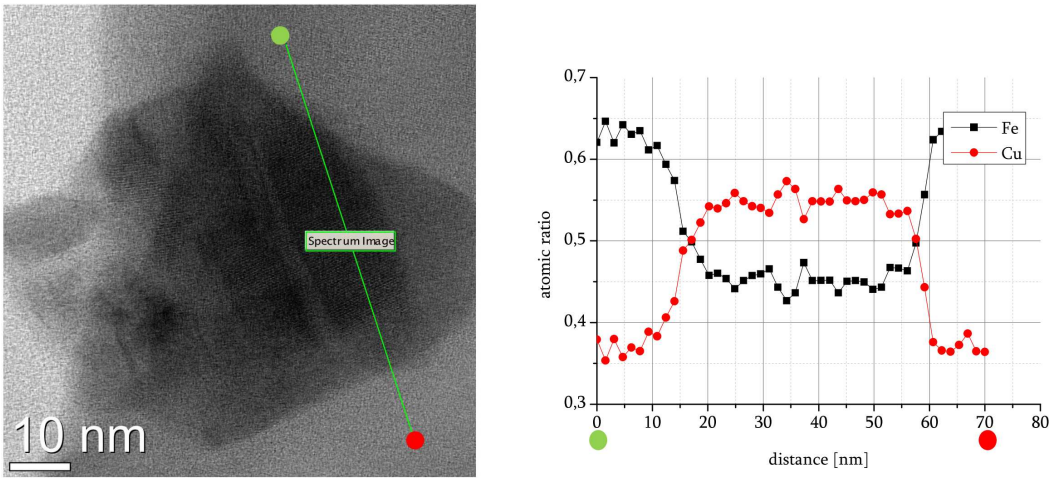

Figure 1: A crystallite of CuO in a $CuFe_2O_4$ matrix (left); Atomic ratio of Cu and Fe from EDX linescan through the crystallite in TEM (right)

As possible mechanisms that contribute to the hindering of ion exchange, the phase transformation accompanied by the formation of thermodynamically stable phases, the clustering of Li ions as well as the formation of strain fields and the modification of the electronic structure in the vicinity of microstructure defects are expected. The experimental work within this subproject is focussed on the microstructure analysis using X-ray diffraction (for the phase analysis, analysis of the crystallite size and microstrain), transmission electron microscopy and electron spectroscopy (for the visualisation of the morphology of crystallites, for the imaging of the Li ion distribution as well as for the local chemical and phase analysis).

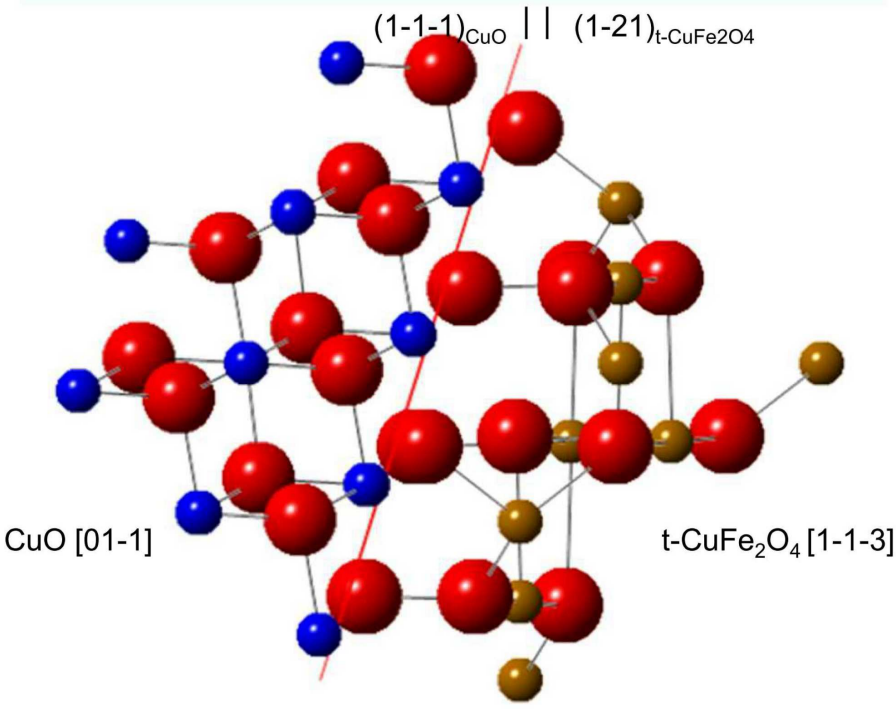

Figure 2: Experimental orientation relationship between CuO and $CuFe_2O_4$ determined by Fourier Transform of High Resolution TEM from area in Figure 1 leads to a partially coherent phase boundary (not in view: $(301)_{\text{t-CuFe2O4}} \parallel (200)_{\text{CuO}}$)