NANOCRYSTALLINE COMPLEX OXIDES PREPARED BY MECHANOCHEMICAL REACTIONS

V. Šepelák^{1.2}, S. Indris¹, K. D. Becker³, W. Bensch⁴, P. Heitjans⁵

¹Karlsruhe Institute of Technology, Karlsruhe, Germany
²Slovak Academy of Sciences, Košice, Slovakia
³Braunschweig University of Technology, Braunschweig, Germany
⁴Christian-Albrechts-University Kiel, Kiel, Germany
⁵Leibniz University Hannover, Hannover, Germany

Among the typical Li ion battery cathode materials, LiFePO₄ of the phospho-olivine family is particularly interesting due to its high energy density, low cost, and environmental compatibility. In the present work, nanocrystalline LiFePO₄ with an average particle size of about 10 nm was prepared via far-from-equilibrium mechanochemical processing of the bulk LiFePO₄ at room temperature. HR-TEM studies revealed a nonuniform structure of LiFePO₄ nanoparticles consisting of an ordered core surrounded by a disordered surface shell/interface region. A comparative ⁵⁷Fe Mössbauer spectroscopic study of bulk and nanocrystalline LiFePO₄ revealed that the near-surface layers of phosphate nanoparticles are disordered due to the strongly distorted geometry of the FeO₆ octahedra. Quantitative information on hyperfine parameters of the nonequilibrium LiFePO₄ phase is obtained.

The work is supported by the DFG in the framework of the Priority Program "*Crystalline Nonequilibrium Phases*" (SPP 1415), and the APVV (0728-07).

Presenting author:	Vladimír Šepelák
Address:	Institute of Nanotechnology, Karlsruhe Institute of Technology,
	Hermann-von-Helmholtz Platz 1, 76344 Eggenstein-Leopoldshafen,
	Germany
FAX:	+49-7247-82-6368
E-mail:	<u>vladimir.sepelak@kit.edu</u>