

Slow Lithium Self-Diffusion on the Nanoscale Studied by Macroscopic and Microscopic Methods

Johanna Rahn¹, Benjamin Ruprecht², Florian Strauß^{1,2,4}, Erwin Hüger¹, Elena Witt², C. Vinod Chandran², Paul Heitjans^{2,3}, Harald Schmidt^{1,3,4}

¹ Institut für Metallurgie, Technische Universität Clausthal, Robert-Koch-Str. 42, 38678 Clausthal-Zellerfeld, Germany; ² Institut für Physikalische Chemie und Elektrochemie, Leibniz Universität Hannover, Callinstr. 3-3a, 30167 Hannover, Germany; ³ Zentrum für Festkörperchemie und Neue Materialien, Leibniz Universität Hannover, Callinstr. 3, 30167 Hannover, Germany;

⁴ Clausthaler Zentrum für Materialtechnik, Technische Universität Clausthal, Leibnizstr. 9, 38678 Clausthal-Zellerfeld, Germany

E-Mail: harald.schmidt@tu-clausthal.de

Fast Li diffusion processes in solids, generally taking place in ion-conductors, are routinely studied in literature due to their importance for battery materials. In contrast, slow diffusion processes are investigated less often. Nevertheless, they are likewise of fundamental interest for understanding material stability (amorphous and nano-crystalline materials) and in order to obtain a coherent general view. In this context, diffusion on short length scales of some nanometers is of special interest due to the given structural peculiarities.

Here, we report on slow Li self-diffusion in lithium containing metal oxide compounds with special emphasis on the influence of structural disorder on diffusion. Case studies on LiNbO₃, LiTaO₃, LiAlO₂, and LiGaO₂ are presented [1–9]. The focus is on comparative studies by macroscopic tracer methods (Secondary Ion Mass Spectrometry, Neutron Reflectometry) and microscopic methods (Nuclear Magnetic Resonance Spectroscopy, Impedance Spectroscopy) on the same type of material.

- [1] Li Self-Diffusion in Lithium Niobate Single Crystals at Low Temperatures, J. Rahn, E. Hüger, L. Dörrer, B. Ruprecht, P. Heitjans, H. Schmidt, Phys. Chem. Chem. Phys. 14 (2012) 2427.
- [2] Diffusivity Determination in Bulk Materials on Nanometric Length Scales using Neutron Reflectometry, E. Hüger, J. Rahn, J. Stahn, T. Geue, H. Schmidt, Phys. Rev. B 85 (2012) 214102.
- [3] Low-Temperature DC Conductivity of LiNbO₃ Single Crystals, B. Ruprecht, J. Rahn, H. Schmidt, P. Heitjans, Z. Phys. Chem. 226 (2012) 431.
- [4] Lithium Diffusion in Congruent LiNbO₃ Single Crystals at Low Temperatures Probed by Neutron Reflectometry, E. Hüger, J. Rahn, T. Geue, J. Stahn, P. Heitjans, H. Schmidt, Phys. Chem. Chem. Phys. 16 (2014) 8670.
- [5] Lithium Diffusion in Ion-Beam Sputtered Amorphous LiAlO₂, J. Rahn, E. Witt, P. Heitjans, H. Schmidt, Z. Phys. Chem. 229 (2015) 1341.
- [6] Li Self-Diffusivities in Lithium Niobate Single Crystals as a Function of Li₂O Content, J. Rahn, P. Heitjans, H. Schmidt, J. Phys. Chem. C 119 (2015) 15557.
- [7] NMR and Impedance Spectroscopy Studies on Lithium Ion Diffusion in Microcrystalline γ -LiAlO₂, E. Witt, S. Nakhal, C. V. Chandran, M. Lerch, P. Heitjans, Z. Phys. Chem. 229 (2015) 1327.
- [8] Unravelling Ultraslow Lithium-Ion Diffusion in γ -LiAlO₂: Experiments with Tracers, Neutrons, and Charge Carriers, D. Wiedemann, S. Nakhal, J. Rahn, E. Witt, M. M. Islam, S. Zander, P. Heitjans, H. Schmidt, T. Bredow, M. Wilkening, M. Lerch, Chem. Mater. 28 (2016) 915.
- [9] Slow Lithium Transport in Metal Oxides on the Nanoscale, J. Rahn, B. Ruprecht, E. Witt, C. V. Chandran, L. Dörrer, F. Strauß, E. Hüger, P. Heitjans, H. Schmidt, Z. Phys. Chem., submitted, 2017.

