

## Lithium Self-Diffusion in Single Crystalline and Amorphous LiAlO<sub>2</sub>

J. Rahn,<sup>1</sup> E. Hüger,<sup>1</sup> E. Witt,<sup>2</sup> P. Heitjans,<sup>2,3</sup> H. Schmidt<sup>1,3</sup>

<sup>1</sup>Institute of Metallurgy, Microkinetics Group, Clausthal University of Technology, Clausthal-Zellerfeld, Germany

<sup>2</sup>Institute of Physical Chemistry and Electrochemistry, Leibniz University Hannover, Germany

<sup>3</sup>Center for Solid State Chemistry and New Materials, Hannover, Germany

Corresponding author: Johanna Rahn, E-Mail: [Johanna.rahn@tu-clausthal.de](mailto:Johanna.rahn@tu-clausthal.de)

Lithium aluminate (LiAlO<sub>2</sub>) is a synthetic crystal with various technological applications. It is used as substrate material for epitaxial growth of III-V semiconductors, in batteries or in fusion reactor technology. In all these cases the stability of the system is correlated to diffusion properties. Therefore, understanding of Li self-diffusion in LiAlO<sub>2</sub> is of fundamental interest.

In order to understand the influence of structural disorder on diffusion, it is especially interesting to study diffusion in different structural states (amorphous, single crystalline) and to compare it to other systems. As previously published for LiNbO<sub>3</sub> [1 - 3], Li self-diffusivities can be higher by at least nine orders of magnitude in amorphous materials compared to single crystals close to room temperature. This dramatic rise in Li mobility is traced back to the introduction of structural disorder. Aim of the present work is to elucidate the situation for LiAlO<sub>2</sub>.

Li self-diffusion studies on sputtered amorphous films and  $\gamma$ -LiAlO<sub>2</sub> single crystals were carried out in comparison using secondary ion mass spectrometry and stable <sup>6</sup>Li isotopes as a tracer source. Amorphous LiAlO<sub>2</sub> films of about 800 nm thickness were prepared by ion-beam sputter coating on sapphire substrates. A <sup>6</sup>LiAlO<sub>2</sub> tracer layer was afterwards deposited on top or alternatively on commercial single crystals. Diffusion annealing was done between room temperature and 473 K on amorphous samples and between 573 and 723 K on single crystals. After diffusion annealing, diffusivities are extracted by fitting appropriate solutions of the diffusion equation to <sup>6</sup>Li isotope depth profiles from SIMS analyses.

The results on  $\gamma$ -LiAlO<sub>2</sub> single crystals are in agreement to extrapolated data from impedance spectroscopy below 520 K as measured in Hannover, giving an activation enthalpy of 1.2 eV. The results on amorphous LiAlO<sub>2</sub> show further that introducing structural disorder has a less tremendous effect on Li self-diffusivity as for LiNbO<sub>3</sub>. Only five orders of magnitude are found in the accessible temperature range. A possible reason might be that the activation enthalpy for the amorphous modification of about 0.9 eV is similar to that of the single crystal, which gives less difference at low temperatures.

The work was done in the framework of the DFG research unit 1277 "molife".

### References

- [1] M. Masoud, P. Heitjans, *Defect Diff. Forum* 237-240 (2005) 1016
- [2] J. Rahn, E. Hüger, L. Dörrer, B. Ruprecht, P. Heitjans, H. Schmidt, *Phys. Chem. Chem. Phys.* **14** (2012) 2427.
- [3] J. Rahn, E. Hüger, L. Dörrer, B. Ruprecht, P. Heitjans, H. Schmidt, *Z. Phys. Chem.* **226** (2012) 439.