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ABSTRACT:

Polaron-Related Chemical Diffusion in Lithium Niobate, LiNbO₃

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The optical absorption spectra of chemically reduced LiNbO₃ (LN) show broad bands in the visible and NIR region which have been attributed to various types of electron small-polarons [1]. At high temperatures, for example at 1000°C, spectra are dominated by an absorption band at about 0.9 eV due to free small-polarons, i.e. to electrons localized on niobium ions on regular sites [1-3]. Band intensity has been found to follow a power-law dependence on oxygen partial pressure P_{O_2} of the form $(P_{O_2})^m$ with $m = -0.23 \pm 0.02$ [2,3]. This m -value is in excellent agreement with the value of $-1/4$ predicted from point defect thermodynamics of the chemical redox model of LN [4]. The polaron-related kinetics of reduction and oxidation of LN have been studied at high-temperature conditions in experiments with rapid changes in oxygen partial pressure which give rise to ambipolar diffusion fluxes of polaronic and ionic defects species. Analysis of these chemical diffusion processes reveals that the relaxation-type experiments can provide a novel route to the determination of diffusion coefficients of lithium vacancies at high temperatures as well as to that of lithium ions.

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[3] J. Shi, H. Fritze, A. Weidenfelder, G. Borchardt, K.-D. Becker, Solid State Ionics 262 (2014) 904

[4] D.M. Smyth, Ferroelectrics, 50 (1983) 93