Preface

This volume of ‘Diffusion Foundations’ comprises several invited chapters about ionic motion and diffusion in ion-conducting materials and thin salt-in-polymer films. The present volume is the second one of two volumes devoted to recent progress in structure, thermodynamics, ion and proton transport in ionic materials. In the present volume oxide ceramic materials and polymer membranes are in focus. Ion conducting, proton conducting and mixed conductor materials are important components of solid state devices for energy storage and conversion and for energy production. The first one of the two volumes appeared with the title ‘Progress in Ion Transport and Structure of Ion Conducting Compounds and Glasses’ as volume 6 of ‘Diffusion Foundations’. The present volume contains five chapters.

Chapter 1 by *Bi-Cheng Zhou and Zi-Kui Liu* is a theoretical paper. It is devoted to modeling techniques of thermodynamic and diffusion properties based on density functional theory and first-principles calculations for ionic materials. For the prediction of thermodynamic and phonon properties at finite temperatures, the frozen phonon and linear response method along with the mixed-space method are used. Thermodynamic and diffusion properties are fundamental information needed for understanding of existing and for designing of new ionic materials. In particular oxide ceramic materials or ion conductor materials are considered in this chapter with a focus on oxides for energy applications.

The focus in Chapter 2 by *Raidar Haugsrud* is on high-temperature proton conductors. Some oxides dissolve protons that are mobile at high temperatures. These materials are essential components in proton conducting solid-oxide fuel cells, in proton conducting solid-oxide electrolyzer cells, and in ceramic hydrogen gas separation membranes. Proton conducting fuel cells rely on high proton conductivity for the electrolyte. Mixed ionic and electronic conductivity are important for the electrodes. Mixed proton-electron conductors are necessary for hydrogen gas separation membranes as well. Such materials are important for energy devices of technologies for green economy. Potential applications and the status of the technologies are briefly discussed in this chapter as well.

Chapter 3 by *Peter Fielitz and Günther Borchardt* considers self-diffusion of alpha-alumina, of mullite – an oxide of aluminium and silicon-, and of alumino-silicate glasses. The constituting elements of these materials are among the most abundant elements in geological materials and are also important for specialized functional materials. The authors use two rare stable isotopes, ^{18}O and ^{30}Si, and the quasi-stable radioisotope ^{26}Al (half-life 74000 a) in combination with SIMS depth profiling to study diffusion properties. These data are relevant for geological as well as manmade materials. The latter comprise a wide spectrum of applications from consumer goods to specialized functional materials.

Chapter 4 by *Harald Schmidt* is a review of Li diffusion in lithium containing metal oxide compounds such as lithium niobate and lithium aluminate. The focus is on tracer studies of Li diffusion. Li ion conductors are important for lithium ion batteries in cathodic materials (such as $LiCoO_2$, $LiMn_2O_4$, $LiNi_{0.33}Co_{0.33}Mn_{0.33}O_2$, $LiFeO_4$), anodic materials (such as $Li_4Ti_5O_{12}$) and solid-state electrolyte materials (such as Li_3PO_4N). Lithium diffusion in components of Li-ion batteries is one of the key parameters, which determines the rate at which a battery can be charged and discharged. These properties are relevant for the power density of batteries. Lithium niobate ($LiNbO_3$) is the most important synthetic oxide. In the field of optics it is sometimes denoted as the ‘silicon of optics’ and has numerous applications in photonics and optoelectronics. A knowledge of Li diffusion is important for its applications in transducers, filters, modulators, lasers, optical waveguides and holographic storage.

Chapter 5 by *Hans-Dieter Wiemhöfer, Steffen Jeschke, and Eva Cznotka* treats ion transport in thin films of salt in polymer electrolytes. Polymer electrolytes are obtained by dissolving an inorganic salt in a polymer matrix. Suitable combinations of polymer s ubstance and a lithium salt may produce solid-like electrolyte materials with properties suitable for battery applications especially for portable applications. Such solid polymer electrolytes combine good ionic conductivity with a high mechanical flexibility but avoid the disadvantages of liquid-like ionic systems.

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