Ionic conduction in glasses and nanocomposite polymer electrolytes CHRISTIAN KARLSSON Department of Applied Physics Chalmers University of Technology Göteborg University

Abstract

This thesis is concerned with experimental studies of ionic conduction in glasses and polymer electrolytes. These classes of materials are of high interest for applications as electrolytes in batteries. However, in order to optimise the performance, a thorough understanding of the ionic conduction mechanisms would be desirable. The present work is concentrated on two aspects of ionic conduction: (1) the structural origin of cation mobility effects that occur when two different cation species are mixed in ion-conducting glasses and (2) the effects of nanoparticle fillers on the structure and polymer dynamics of polymer electrolytes.

The microscopic structure and conductivity properties of various glass systems containing two or more cation species that potentially are mobile were investigated using diffraction techniques, reverse Monte Carlo modelling and dielectric spectroscopy. The aim was to understand the mixed alkali effect and related phenomena. A structural model of mixed alkali Li-Rb phosphate glasses is proposed, from which the mixed alkali effect qualitatively can be understood. In mixed alkali alkaline-earth glasses the structure provides explanations for some unusual effects on ion mobilities that occurs on mixing. In CsI-doped AgPO₃ glasses the conductivity is shown to be determined by different factors with origin in the glass structure. Furthermore, a dielectric spectroscopy study of LiPO₃ covering a wide frequency range (mHz to GHz) shows that conductivity spectra measured in the temperature range 120–400 K follow a scaling behaviour. The scaling relation provides clues for the underlying conductivity mechanism and also a critical test for theories that are suggested to explain ion-conduction in glasses.

Nanocomposite polymer electrolytes, consisting of polymer, salt and inorganic filler particles were investigated using neutron scattering with the aim to clarify the origin of the enhanced conductivity observed on addition of filler in these systems. The results show that the polymer dynamics is reduced when filler is added and that the filler particles form fractal, polymer-like chain structures in the polymer electrolyte. The results provide dynamical and structural support for a previous suggestion that the conductivity increase is due to the formation of conducting percolating surface layers.

Keywords: ionic conduction, glasses, mixed alkali effect, polymer electrolytes, nanocomposites, polymer dynamics, dielectric spectroscopy, neutron diffraction, quasi-elastic neutron scattering, QENS, x-ray diffraction