A computer simulation study of ionic conductivity in polymer electrolytes

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Abstract. In this paper we present a computer simulation study of ionic conductivity in solid polymeric electrolytes. The multiphase nature of the material is taken into account. The polymer is represented by a regular lattice whose sites represent either crystalline or amorphous regions with the charge carrier performing a random walk. Different waiting times are assigned to sites corresponding to the different phases. A random walk (RW) is used to calculate the conductivity through the Nernst–Einstein relation. Our walk algorithm takes into account the reorganization of the different phases over time scales comparable to time scales for the conduction process. This is a characteristic feature of the polymer network. The qualitative nature of the variation of conductivity with salt concentration agrees with the experimental values for PEO–NH_4I and PEO–NH_4SCN. The average jump distance estimated from our work is consistent with the reported bond lengths for such polymers.

1. Introduction

During the last two decades a lot of interest has been generated in the potential industrial applications of polymer electrolytes [1,2]. Hence, developement of theoretical understanding of such materials is essential. Polymeric solid electrolytes are formed by complexing an ionic salt like NaI, NH_4SCN, etc with polymers, for example polyethylene oxide (PEO), polypropylene oxide (PPO), [3,4] etc. We restrict our discussion to solvent free polymer electrolytes which are formed by dissolving or suspending the salt and the polymer in a suitable solvent and then evaporating the solvent during casting.

The theoretical explanation of the dependence of ionic transport on temperature, salt fraction, frequency, etc. is a formidable problem. The complications arise mainly because these polymer systems are multiphase in nature. Further difficulties creep in because the presence of different phases are dependent on processing conditions and thermal history.

The aim of this work is to study the variation of ionic conductivity in a polymer electrolyte where the salt fraction is varied. The varying salt fraction changes the proportion of crystalline and amorphous regions and also the concentration of charge carriers supplied by the salt [5].

The final goal is of course to predict the conductivity of an unknown polymer complex with a given salt fraction. In this work we have not fully achieved this since