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Numerical simulation of ion distribution in polymer electrolytes with blocking electrodes

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ABSTRACT

A numerical procedure is introduced to calculate the profiles of ion densities and electric fields in polymer electrolytes with blocking electrodes. For low electric potentials the numerical results are in agreement with Jaffé's approximate analytical solutions. In contrast to the analytical solution the numerical procedure is also suitable for high electric potentials at which the relation between dielectric polarisation and electric potential becomes strongly nonlinear. Furthermore, the temporal development of ion distributions can be modelled after the application of a voltage step or under other transient voltages.

1. Introduction

Polymer electrolytes are of significant technological interest because of their potential for use in batteries, membranes for fuel cells, and sensors. With suitable combinations of polymers and an alkaline salt a solid-like electrolyte with sufficient ionic conductivity may be produced [1]. It is believed that understanding the ionic transport mechanism will aid the optimisation of future polymer systems [2]. For this reason the motion of ions in a polymer matrix is a very interesting topic.

Ionic motion shows effects in the low frequency region, where moving ions contribute significantly to the overall current during one half-period of a harmonic excitation. For this reason, studying conduction at such frequencies and comparing with theory is an important tool. In the present work, a numerical calculation for time dependent ion distributions under external electric potentials is introduced.

2. Theory

Moveable ions in polymer electrolytes are often unable to cross material-electrode boundaries. If low frequency voltages are applied on the electrodes, large concentrations of ions develop near those interfaces. This effect was firstly treated theoretically based on Maxwell's theory by Wagner [3] and Sillars [4], leads to large dipole moments since oppositely charged ions propagate to opposite ends of the sample.

The ions' distribution in a homogeneous material in such cases is a result of drift and diffusion and, assuming a constant number of ions, is described in one dimension by Jaffé G [5]:

$$\frac{\partial p}{\partial t} = D_p \frac{\partial^2 p}{\partial x^2} - \mu_p \frac{\partial}{\partial x}(pE) \tag{1}$$

$$\frac{\partial n}{\partial t} = D_n \frac{\partial^2 n}{\partial x^2} + \mu_n \frac{\partial}{\partial x}(nE) \tag{2}$$

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