Monte Carlo simulation of a 3D solid electrolyte on a simple cubic lattice: concentration and electric field distribution at and without an external field

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Solid electrolytes are widely used in rechargeable batteries, fuel cells, supercapacitors, to name a few. Accounting for long range Coulomb interactions is one of the challenges in their theoretical investigations. Additional difficulties appear due to their ceramic structure and presence of intergrain boundaries.

A three-dimensional (3D) model of a solid electrolyte is considered. It consists of a one-component electrolyte on a 3D simple cubic lattice with neutralizing static background. In addition to Coulomb interactions a short-range van der Waals interactions are taken into account. The ions perform thermally activated hops to vacant nearest neighbor lattice sites. The structural peculiarities of the system are reflected by an energetic landscape. The intergrain and near electrode regions are modelled by variations of site and intersite energies.

Monte Carlo simulations were performed for calculating the charge and concentration distribution at various thermodynamic conditions. The Ewald summation was used for accounting for the Coulomb interactions. The electric current and conductivity were estimated at open circuit conditions by the number of ions passed through the system.

The simulation results has allowed investigating the structure of electric double layers in intergrain and near electrode areas. They are compared with the results of more simple quasi-one-dimensional models [1,2].

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[2] T. Patsahan, G. Bokun, D. di Caprio, M. Holovko, V. Vikhrenko, Solid State Ionics 335 (2019) 156.