Structure at Electrified Interfaces

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Molecular Dymanics simulations of a molten salt, KCl, confined between charged walls have been performed using the rigid ion model. We use a Fumi-Tosi type potential with the long range electrostatic interactions handled by a 2D Ewald summation. The structure and dynamics of the ions have been investigated along with the charge density and potential across the cell at a number of different temperatures and wall charges. Whilst in simulations with large wall charges there is significant polarisation in the melt, there has been no sign of crystallisation in the ion layers adjacent to the walls. Comparisons of the potential and charge density show there is a linear drop in the potential over the first ion layer whereas fluctuations in the charge density extend much further from the walls.