A thermodynamic perturbation theory for the surface tension and ion density profile of a liquid metal

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Abstract

Assuming that the interaction between metallic pseudo-ions is of the form introduced by Evans (1974, 1975), an approximate expression for the excess free energy of the system is derived using the thermodynamic perturbation theory of Weeks, Chandler and Anderson (1971). This excess free energy is then minimized with respect to a parameter which specifies the ion density profile, and the surface tension is given directly. From consideration of the dependence of the interionic forces on the electron density it is predicted that the ions should take up a very steep density profile at the liquid metal surface. The values of the surface tension calculated for liquid Na, K and Al from a simplified version of the theory are in reasonable agreement with experiment.