Lattice-Gas Model for Cl on Ag(100) Single-Crystal Surfaces

Ibrahim Abou-Hamad,[1] Per Arne Rikvold,[1] Steven J. Mitchell[2] and Thomas Wandlowski[3]

[1]Florida State University
Department of Physics, Center for Materials Research and Technology, and School of Computational Science and Information Technology
Tallahassee, FL 32306-4350
USA

[2]Eindhoven Technical University
Department of Chemical Engineering and Chemistry
ST W.3.42
Eindhoven 5612 AZ
The Netherlands

[3]Forschungszentrum Jülich
Institut für Grenzflächenforschung
Jülich D-52425
Germany

We report on a new lattice-gas model for the adsorption of Cl on Ag(100) single-crystal electrodes. The model is similar to one previously developed for Br on Ag(100) [1-3], with nearest-neighbor exclusion and long-range $1/r^3$ repulsive interactions. The strength of the long-range interaction is estimated by fitting equilibrium Monte Carlo simulations to data from chronocoulommetry experiments. The Monte Carlo simulations utilize an optimized method for calculating the long-range interactions, in which the energy contributions from close neighbors are calculated exactly, while contributions corresponding to larger adparticle separations are calculated in a mean-field approximation.

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