IOP PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **19** (2007) 305006 (10pp) doi:10.1088/0953-8984/19/30/305006

# Diffraction patterns of He atoms from the MgO(100) surface calculated by the close-coupling method

**R Martínez-Casado[1,2], B Meyer[3], S Miret-Artés[2], F Traeger[1] and Ch Wöll[1]**

[1] Lehrstuhl für Physikalische Chemie I, Ruhr-Universität Bochum, D-44780 Bochum, Germany
[2] Instituto de Matemáticas y Física Fundamental, Consejo Superior de Investigaciones Científicas, Serrano 123, 28006 Madrid, Spain
[3] Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany

E-mail: ruth@imaff.cfmac.csic.es

Received 5 February 2007, in final form 13 March 2007
Published 13 July 2007
Online at stacks.iop.org/JPhysCM/19/305006

**Abstract**

An analysis of He diffraction data for the MgO(001) surface which goes beyond hard-wall eikonal approximations is presented. In a first step, a model potential, for which the form of a corrugated Morse potential is chosen, is set up using the eikonal approximation in connection with an effective corrugation function. The obtained corrugation amplitude is compared to results from density-functional theory calculations of the He–MgO interaction. In a second step, this model potential is used for close-coupling (CC) calculations of He diffraction intensities. A kinematical analysis of the system He/MgO is given. The results on the He diffraction intensities are in good agreement with the experiment.

(Some figures in this article are in colour only in the electronic version)