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

R Martínez-Casado1,2, B Meyer3, S Miret-Artés2, F Traeger1 and Ch Wöll1

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)

1. Introduction

In recent years the number of studies on oxide surfaces has largely increased and several review articles have been published [1–6]. Despite very careful investigations and optimized methods, inherent problems remain: oxides are insulating materials, for which all methods using or producing electrons are frequently hampered by artifacts due to charging or due to damage produced by impinging electrons. In some cases, the use of very low electron currents, nowadays available e.g. in channel plate low-energy electron diffraction (LEED) systems, reduces these artifacts. In other cases, for instance ZnO or TiO2, a conduction mechanism via defects sets in and facilitates the use of scanning tunnelling microscopy (STM), LEED and other well-developed standard techniques [3]. Except for the cleavage faces of the rocksalt-type oxides, MgO, NiO and CoO [7–15], on most oxide surfaces usually a comparatively large defect density is present, which decreases the reliability of methods which cannot distinguish