He atom scattering from ZnO surfaces: calculation of diffraction peak intensities using the close-coupling approach

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Abstract
Diffraction intensities of a molecular He beam scattered off the clean and water-covered ZnO(1010) surface have been simulated using a new potential model in conjunction with the close-coupling formalism. The effective corrugation functions for the systems He–ZnO(1010) and He–H2O/ZnO(1010) have been obtained from density functional theory calculations within the Esbjerg–Nørskov approximation. Using these data a potential model is constructed consisting of a corrugated Morse potential at small He–surface distances and a semiempiric attractive part at larger distances. The diffraction patterns obtained from close-coupling calculations agree with the experimental data within about 10%, which opens the possibility to simulate He diffraction from surfaces of any structural complexity and to verify surface and adsorbate structures proposed theoretically by employing this kind of analysis.

1. Introduction
He atom scattering is a very sensitive tool for the analysis of surface structures, since it employs neutral and slow probe particles with incident energies in the range of 10–80 meV. Therefore, it combines the advantages of non-destructiveness and absolute sensitivity to the topmost layer [1–4]. Additionally, the scattering cross section between He atoms and surface defects is large, so that nearly all detectable signal stems exclusively from coherent scattering from the periodically ordered parts of the surface. A further strength of He atom scattering is its sensitivity for hydrogen atoms [5], which are hard to detect by most other diffraction techniques. Beyond structural investigations, it is also possible to measure adsorbate dynamics by inelastic scattering [6] and to obtain information on the He–surface interaction potential [7].

In particular for oxide surfaces these prerequisites are beneficial, since most oxides are poor conductors and sometimes surface preparation and cleaning is tedious. He scattering experiments have been performed on cleavage faces of NiO, CoO and MgO, as well on ZnO, TiO2 and KTaO3, which have more complex surface structures; see [4] and references therein.

Relying on a diffraction technique, however, requires a conversion of the information gained in reciprocal space to real space structures. This is usually done by comparing calculated diffraction intensities for model structures with the