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Surface Science 109 (1981) 419-434 North-Holland Publishing Company

SPIN POLARIZATION IN LOW-ENERGY ELECTRON DIFFRACTION: SURFACE ANALYSIS OF Pt(111)

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Received 2 February 1981

Transverse and longitudinal spin polarization components arising in the diffraction of unpolarized low-energy electrons from Pt(111) have been studied as functions of energy and diffraction geometry. Experimental data measured by means of a Mott detector are in good agreement with theoretical results obtained by relativistic LEED calculations. A detailed investigation of the selective sensitivity of the calculated polarization profiles to the surface relaxation δ_{12} and to various non-structural model features firstly supports an ion-core potential involving an energy-dependent exchange approximation (by discriminating against two band structure potentials), and secondly establishes the geometry of Pt(111) as unreconstructed with a possible slight outward relaxation of the topmost atomic layer ($\delta_{12} = 0.5\% \pm 1.0\%$ of the bulk interlayer distance). A surface Debye temperature is found close to the bulk value 230 K.

Surface Science 109 (1981) 435-443 North-Holland Publishing Company

THEORETICAL STUDIES OF THE ANGULAR DISTRIBUTIONS OF OXYGEN ATOMS EJECTED FROM AN ION BOMBARDED $c(2 \times 2)$ OVERLAYER OF OXYGEN ON Ni(001)

II. Effect of interaction potential

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Received 11 March 1981

A detailed molecular dynamics study has been performed in order to determine the influence of the interaction potential on the angles of ejection of oxygen atoms from an ion bombarded $c(2 \times 2)$ oxygen overlayer on Ni(001). The bonding site of the adsorbate appears to be the dominating factor which influences the angles of ejection. Changing the interaction potential affects the angular distribution similarly to varying the height of the adsorbate above the surface.

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