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SIMPLE APPROACH TO REFRACTION EFFECTS IN ATOM–SURFACE SCATTERING

J.G. MANTOVANI and J.R. MANSON

Department of Physics and Astronomy, Clemson University, Clemson, South Carolina 26631, USA

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A simple method of calculating low energy atom–surface diffraction intensities is presented for the case in which the scattering is dominated by a single rainbow pattern. Good agreement is obtained when these calculations are compared with recent results for the scattering of He by a Pt(997) surface.

Low energy atom diffraction has proven itself to be very useful in the interpretation of surface structure for a variety of systems [1]. Much current work is involved with metal surfaces and in particular significant advances have been made in understanding the nature of stepped metal surfaces [2,3]. Of recent experimental and theoretical interest is the scattering of a low energy monoenergetic He beam from the (997) stepped surface of platinum and the interpretation of these data using a corrugated hard wall model [4]. In the experiment a 16.3 meV monoenergetic beam of helium atoms is directed toward the (997) platinum surface in the "step-down" or "downstairs" direction with the beam perpendicular to the step edges. In this configuration there are virtually no beams diffracted out of the plane of incidence since the surface is very smooth in the direction parallel to the step edges, and the problem is essentially that of a one-dimensional corrugated surface. Experiments were carried out over a large range of incident angles and in each case the diffraction consisted of a well defined rainbow pattern of about three significant peaks in the direction specular to the flat step terraces, and very little, if any, intensity in the direction specular to the surface. The data were interpreted in terms of a corrugated hard wall model which included an adsorption well having the correct $-C/z^3$ asymptotic behavior and with a corrugation profile made up of straight line segments to match the triangular steps. Quite resonable agreement was obtained between experiment and the theoretically predicted peak heights and in the process an adsorption well depth of approximately 4 meV was found to give the best agreement.

In this paper we present an alternative method of interpreting the experimental results which has the advantage that it is much simpler and faster than the exact method described above yet still gives identical quantitative results. We chose to represent the surface repulsion by a corrugated hard wall, but instead of an exact calculation, we use an eikonal approximation of the type developed by Garibaldi et al. [5]. We also assume that the only significant function of the attractive well is to "refract" the particles by changing the normal momentum and hence the direction of the incoming beam with respect to the surface, i.e. the attraction is modeled by a square well and all back-scattering by the front edge of the well is ignored. In addition we find that it is sufficient to use a hard wall corrugation function of triangles made up of straight line segments, smoothing effects at the step edges make very little change in the diffracted intensities.

The eikonal approximation is generally valid when all of the important diffracted beams emerge very near to the surface specular. However, we would like to point out that the simplest eikonal approximation should be equally valid when nearly all of the diffracted intensity is scattered within any small solid angle (e.g. a rainbow direction) as in the case of the experiments under discussion here. The eikonal approximation is most easily obtained from the Rayleigh ansatz that the wave function can be expressed in terms of an incident beam plus outgoing scattered beams

$$\psi = e^{-ik_{0z}z}\, e^{i\boldsymbol{K}_0\cdot\boldsymbol{R}} + \sum_{\boldsymbol{G}} A_{\boldsymbol{G}}\, e^{i(\boldsymbol{K}_0+\boldsymbol{G})\cdot\boldsymbol{R}}\, e^{ik_{Gz}z}, \tag{1}$$

where z is the surface normal, $\boldsymbol{R}$ is the position vector parallel to the surface, a wave vector is written as $\boldsymbol{k}_l = (\boldsymbol{K}_l, k_{lz})$, $\boldsymbol{G}$ is a reciprocal lattice vector, and energy conservation implies $k_{Gz}^2 = K_0^2 + k_{0z}^2 - (\boldsymbol{K}_0 + \boldsymbol{G})^2$. The wave amplitudes $A_{\boldsymbol{G}}$ are specified by the condition $\psi = 0$ on the surface:

$$0 = 1 + \sum_{\boldsymbol{G}} A_{\boldsymbol{G}}\, e^{i\boldsymbol{G}\cdot\boldsymbol{R}}\, e^{i(k_{Gz}+k_{0z})\phi(\boldsymbol{R})}, \tag{2}$$

where $\phi(\boldsymbol{R})$ is the corrugation function. If all the important diffracted beams are scattered very close to a single direction denoted by $\boldsymbol{G} = \boldsymbol{F}$ (or more precisely if $k_{Gz} \simeq k_{Fz}$ for all beams with non-negligible intensity) eq. (2) simplifies and after a Fourier transformation gives for the scattered wave amplitudes $A_{\boldsymbol{G}} \simeq A_{\boldsymbol{G}}^{00}$ where

$$A_{\boldsymbol{G}}^{00} = -\frac{1}{S}\int_{\text{u.c.}} d\boldsymbol{R}\, \exp\{i[\boldsymbol{G}\cdot\boldsymbol{R} + (k_{Fz} + k_{0z})\,\phi(\boldsymbol{R})]\}. \tag{3}$$

The usual case to which this expression is applied is when all of the diffraction is near specular and $k_{Fz} = k_{0z}$, but for the case at hand we choose k_{Fz} to correspond to the direction of rainbow scattering from the step terraces.

We also mention in passing that eq. (3) with k_{Fz} replaced by k_{Gz} is the most general eikonal approximation and is obtained by neglecting off-diagonal elements in the matrix equation generated by the Fourier transformation of eq.

(2). For calculations carried out below we label the scattering amplitude calculated in this manner as A_G^0. In all cases the diffracted intensities are given by

$$I_G = \cos\theta_G |A_G|^2 / \cos\theta_0, \tag{4}$$

where θ_G is the angle of the diffracted beam corresponding to $\boldsymbol{G}$.

The most important effect of the adsorption well in front of a metal surface is the possibility of resonant scattering with the bound states, historically called selective adsorption. In circumstances where there are no observed resonances, such as the experiments of refs. [3] and [4], the most important effects of the well are to change the direction of the incoming and scattered particles (a refraction effect in semiclassical terms) and to cause the particle to collide with the repulsive potential at a higher effective kinetic energy. We have accounted for these effects in the simplest possible manner by assuming a one-dimensional square well of depth D in front of the corrugated hard wall and ignoring the effects of scattering by the attractive front edge, i.e. in calculating A_G for example, by eq. (3) k_{Gz} is replaced by $(k_{Gz}^2 + 2mD/\hbar^2)^{1/2}$. This approximation has been used previously with reasonable success [6] and the approximation of neglecting scattering by the front edge is justified by the fact that a realistic potential would be slowly varying in that region and would give rise to very little backscattering.

The profile $\phi(\boldsymbol{R})$ is chosen as two straight line segments making a triangle with the surface plane. This makes eq. (3) an elementary exercise to integrate. The segment corresponding to the step terrace makes an angle of 6.45° with respect to the surface and the step face makes an angle of 20°, this latter choice being made to agree with the best fit for a Cu(117) surface [7].

The results of the calculations are shown on fig. 1 together with the experiment and model calculations of ref. [4]. It is clear that intensities calculated from the amplitude A_G^{00} of eq. (3) or from the slightly more sophisticated approximation A_G^0 are virtually identical with those of the exact calculations. A value of 4 meV seems to be a close estimate of the well depth although the calculation for 3.5 meV seems to indicate that the well depth may be somewhat smaller. A depth smaller than 4 meV gives better agreement at more normal incidence angles and perhaps less good near glancing incidence. However, at glancing incidence the eikonal approximation fails and the experiments are also generally much more difficult to interpret.

We have considered the effects of varying the angle of the step face from 20° but as expected this has a very small effect due to the "step down" scattering configuration. Effects of rounding the sharp corners of the profile are also small, in particular they do not strongly affect the intensity of the specular peak as might be expected. Debye–Waller (or thermal) attenuation is also negligible due to the close angular spacing of the important diffraction peaks.

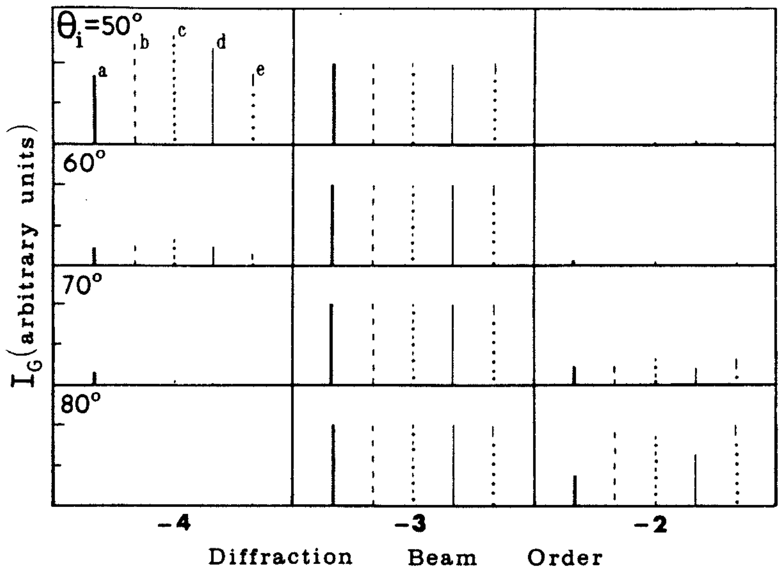

Fig. 1. Diffracted beam intensities for the scattering of a 16.3 meV He beam by a Pt(997) stepped surface: (a) experiment of ref. [4]; (b) calculations of ref. [4] with $D=4$ meV; (c) present calculations using A_G^0 with $D=4$ meV; (d) present calculations from A_G^{00} of eq. (3) with $D=4$ meV; (e) present calculations from A_G^{00} with $D=3.5$ meV.

In conclusion, the comparisons of experiment with theory show, as has been demonstrated many times recently [1], that low energy atomic surface scattering can be a powerful tool in obtaining information on surface structure and the surface potential. This paper demonstrates a class of situations in which important information can be obtained with a very simple theoretical approach and in which no more than a hand calculator is needed to perform the computations.

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