Surface Science 80 (1979) 24–31

STRUCTURE OF THE Ag(110) SURFACE DETERMINED BY USING AVERAGED LEED INTENSITIES

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The constant momentum transfer averaging method has been used to determine the surface structure of the Ag(110) surface. A contraction of 8% of the first layer spacing compared to the bulk value is found by comparing the shape of the averaged intensity profiles with kinematic calculations rather than the position of the peaks. This result agrees well with that obtained by a multiple scattering calculation.

1. Introduction

Since the constant momentum transfer averaging (CMTA) of LEED data was first proposed by Lagally, Ngoc and Webb [1] rather few applications of this method have been published. A few clean, nearly unreconstructed surfaces have been studied [2–5] which mainly show that the averaged intensities have indeed a kinematic behaviour. Differences in the phases of effective scattering amplitudes of adsorbate and bulk atoms may lead to erroneous layer spacings on account of multiple scattering effects which do not completely vanish by averaging as Pendry has shown [6]. Therefore, the determination of adsorbate structures seems to be more difficult [7]. Recently a study of the hydrogen stabilized Si(100) surface has been published [8], the results of which indicate a concentration of the first layer spacing. The results of the reconstructed Si(100) (2×1) surface [8] also seems to be useful in structure determination, but could not yet be successfully interpreted. No quantitative determination of the structure of reconstructed surfaces has yet been done using the CMTA method. A different averaging procedure has been applied by Aberdam et al. [9] to the Al(110) surface, and a direct evaluation of LEED intensities has been done by Chan et al. [10] leading to the same results as dynamical calculations. The results presented here for the Ag(110) surface also agree well with dynamical calculations [15,19] and show that averaged LEED intensities of clean reconstructed metal surfaces can be quantitatively interpreted. The computer time and space needed for the data analysis is negligible compared

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to a multiple scattering calculation and the large amount of data which is necessary does not cause any problems as the data collection can be done automatically.

2. Experimental

The LEED apparatus consists of a four-grid display screen with electron gun and Faraday cup movable in front of the screen. The system has been described in detail elsewhere [11].

The Ag sample – 99.999% (5N) purity from Metals Research Ltd. (England) – was mounted on a two-circle goniometer and cut within 0.5° from a (110) plane by spark erosion and was mechanically and chemically polished in the same way as described by Bradshaw et al. [12]. Afterwards the crystal was cleaned in the UHV system by alternating argon ion bombardment and short heating up to 450°C until no impurities could be detected in the Auger spectrum. The main impurity was sulphur, and up to 20 cycles of ion bombardment and heating were necessary to achieve that no more sulphur segregated to the surface during the final annealing at 300°C for several hours. The temperature and duration of annealing were chosen such that the half-widths of the LEED beams were minimized. However, the background intensity was higher and the LEED beams remained somewhat broader than those of a (100) surface of the same specimen. This behaviour indicates that the (110) face is less stable and contains more surface defects than the other low index faces of silver. Similar results have been reported in different studies of the Ag(110) surface [12–14].

To render manageable the large amount of intensity data necessary for averaging both, the movement of the Faraday cup in one direction and the data collection were computer controlled. The intensities of the specular beam were measured between 20 and 700 eV in steps of 2 eV below 200 eV, and 4 eV above respectively. The angle of incidence was $16° \leqslant \vartheta \leqslant 60°$, where 0° refers to normal incidence, and was varied in steps of 2°. These measurements were made for three different azimuths, $\phi = 0°$, 10°, where 0° corresponds to the $(1\bar{1}0)$ direction. As has been mentioned earlier by several authors [2,5,7], the results of the averaging method are improved by including the whole range and a finer mesh of azimuthal angles. For technical reasons this was not possible during this study but we believe that the error in the layer spacings is essentially due to the limited range in azimuthal angles.

For comparison with multiple scattering calculations the intensities of six non-specular beams at normal incidence were also measured. A detailed description of the experimental procedure and of all experimental results is given in ref. [11].

3. Results

The averaged intensity profile of the specular beam is shown in fig. 1 on a linear and on a logarithmic scale. The relatively small interlayer distance of the (110)

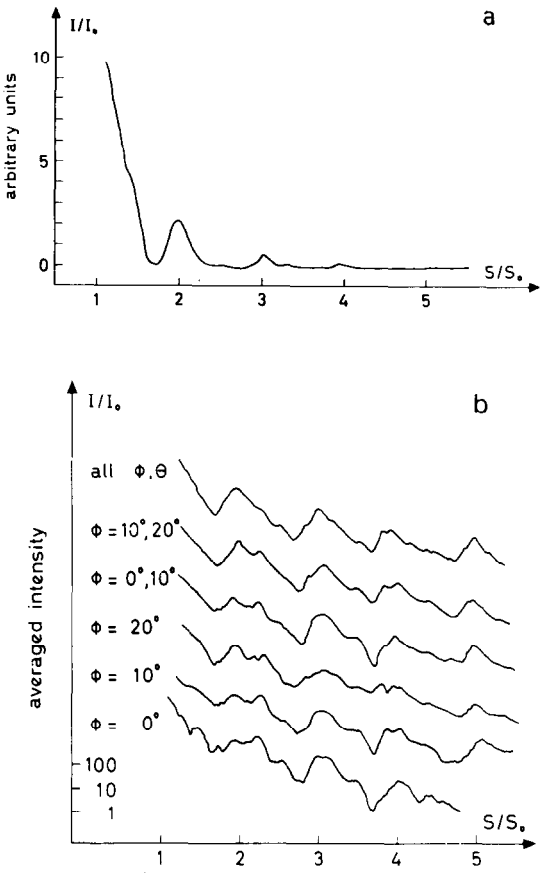

Fig. 1. (a) Experimental intensity profile of the specular beam. The average was performed for $16° \leqslant \vartheta \leqslant 60°$, $\Delta\vartheta = 2°$, and $0° \leqslant \phi \leqslant 30°$, $\Delta\phi = 10°$. (b) Upper curve same as above on a logarithmic scale. The averages in the lower curves were performed for one or two azimuth angles as indicated in the figure.

planes requires energies up to 700 eV to observe the higher order reflections and the intensity of these is strongly reduced by the low Debye temperature of silver. Therefore, the logarithmic scale is much better suited for comparison with the calculated curves. In fig. 1b also the curves are shown in which a smaller set of measurements was averaged. There remains a rather large amount of multiple scattering structure when the average does not include all azimuth angles ϕ. Only the upper curve is compared with the calculations and obviously the result could be improved by including the whole range of aximuth angles. The theoretical curves have been calculated kinematically, using the atomic scattering factor and were

then averaged in the same way as the experimental curves.

Only the first layer spacing has been varied in the calculations, and a comparison with the experimental curve indicates a contraction of about 8%, the error can be estimated to be about 2%. The real part of the inner potential has been found to be 10.5 eV by comparison with dynamical calculations using the same phase shifts, and the imaginary part has been set to $V_i = 4$ eV. This inner potential has been corrected as proposed by Pendry [6] to take into account those multiple scattering processes depending on $S = k - k'$ which do not vanish by averaging in the CMTA method and which can be related to zero angle scattering. The correction part is constructed by:

$V_F = f(\vartheta = 0, E)/\Omega$, Ω is unit volume per atom.

That means, a constant potential is added which gives the desired forward scattering. Fig. 3 shows the real and the imagniary part of the correction term. The additional damping is necessary to match the experimental peak widths, which are distinctly broader than the kinematically calculated ones. In the procedure described by Lagally et al. [1] an adjustable damping parameter has been added to produce the required peak widths. However, the calculations of a correction term according to Pendry is quite easy and work well without further adjustment.

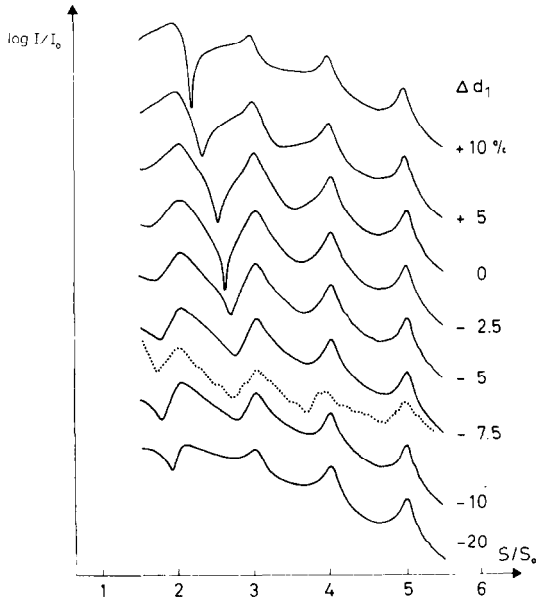

Fig. 2. Averaged intensities of the (00) beam of Ag(110). Dotted line: experiment; full line: calculated averages. Δd_1 denotes the relaxation of the top layer spacing.

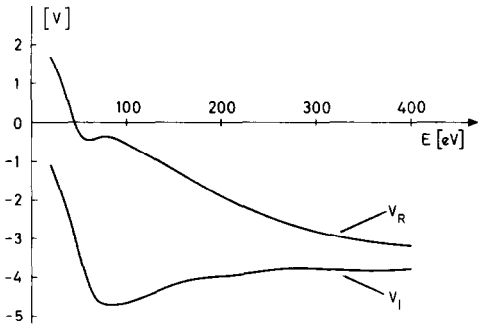

Fig. 3. Real V_R and imaginary part V_i of the correction term to the inner potential as proposed by Pendry [6].

A surface Debye temperature $\theta_S = 140$ K has been assumed for the first layer, and a bulk value $\theta_B = 225$ K for all other layers in the kinematic calculations. Though the incident electron wave is rather strongly damped it has been found necessary to take into account about ten layers to reach convergence in the calculations. The number of phase shifts which is necessary to give a correct description of the atomic scattering factor increases rapidly with increasing energy; up to 15 phase shifts have been used. Nevertheless, the influence of the number of phase shifts on the averaged intensity profiles has been tested too and the result is shown in fig. 4.

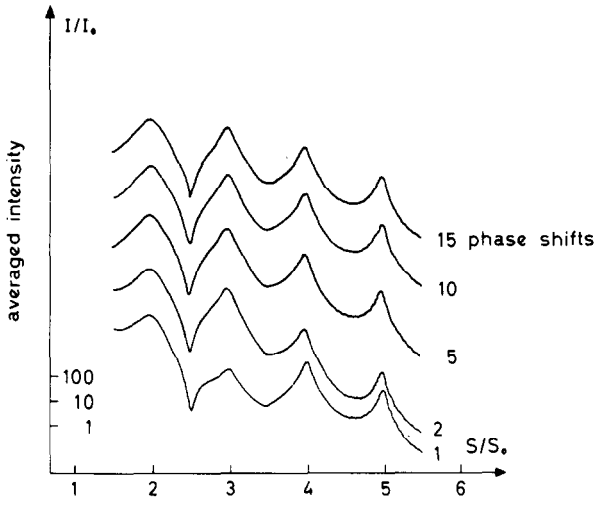

Fig. 4. Influence of the number of phase shifts used in the kinematic calculation of averages for the unreconstructed surface.

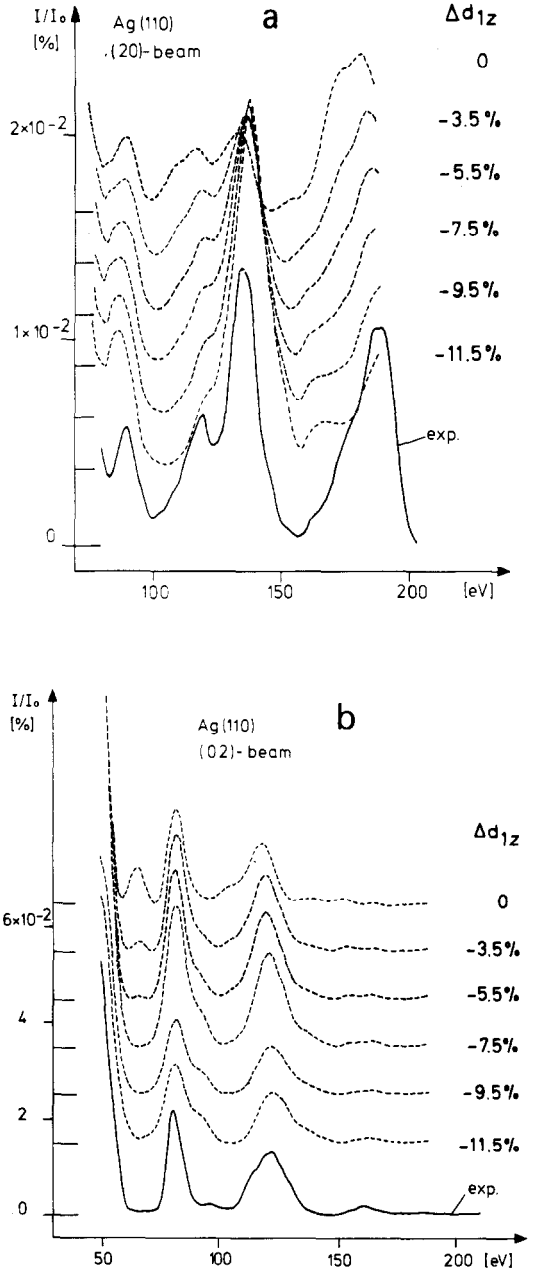

Fig. 5. Comparison between experimental (full line) and calculated intensity profiles (dashed line). Δd_1 denotes the contraction of the first layer spacing. Seven phase shifts were used and the bulk Debye temperature $\theta_B = 225$ K was assumed for all layers.

The averaged profiles are obviously very insensitive to changes in the scattering factor; two phase sifts are nearly sufficient. The shape of the intensity profiles is solely determined by the surface geometry.

For comparison with an exact multiple scattering calculation six beams at normal incidence have been measured; two of them – when small changes in surface geometry affect the intensity profiles rather strongly – are shown in fig. 5. Visual comparison between all theoretical and experimental curves lead to the same contraction of the first layer spacing of about 8% as the averaging method [19]. A detailed study of the Ag(110) surface, using an R-factor analysis in the comparison of calculated and experimental curves, has been published recently by Maglietta et al. [15]. These authors report a slightly greater concentration of about 10% which is within the error limit of this study.

The multiple scattering calculations were done using the RFS scheme of Pendry [17] and the phase shifts were constructed using a superposition of Hartree potentials obtained from the Herman–Skillman atomic wave functions and an energy dependent approximation to the exchange term as described by Slater, Wilson and Wood [18]. A similar potential for silver has been used by Forstmann [16] in calculations for the Ag(111) surface and also gave very good results for the Ag(100) surface [19].

4. Discussion

Variation of just one layer spacing causes only very small shifts of the peak positions in the averaged intensity curve of the 00 beam while their shape is much more affected. Introducing a smaller distance causes a shoulder in the peak on the high energy side and the bulk distance interferences remain mainly unchanged; only a small shift due to the asymmetry of the peak occurs. The influence of the variation of the top layer spacing is best seen on a logarithmic scale as shown in fig. 2. As expected, this influence weakens at higher energies due to the increasing penetration depth of the incident electrons. The main effect is visible between the first two orders of diffraction, and this region can be compared with the experiment. No attempt has been made to determine the layer spacings from the peak positions, nor have we tried to vary the next layer spacings as the effects are too weak to be detected.

One of the objectives of the averaging method is to determine the atomic distances in the surface more precisely when compared with multiple scattering calculations. In a multiple scattering analysis some incertainties remain, those are mainly due to the potential used in the calculation. Calculations with different potentials may lead to slightly different results, an effect which one tries to overcome by comparing a large number of beams.

Secondly, for comparison with multiple scattering calculations the intensities of the beams have to be measured very carefully with respect to angles of incidence,

since small errors in the orientation of the incident beam may cause rather large errors in the measured intensities.

In the averaging method this effect is less important and also the influence of the potential in the calculated curves does not seem to be relevant as can be seen quite clearly from fig. 4. Among the nonstructural parameters only the inner potential seems to be important in the averaging method. An overall shift of the inner potential shifts the peak positions only, leaving their shapes nearly unchanged (not quite, as an angular dependence exists due to refraction of the incident beam), whereas a lowering of the real part of the inner potential between the first two or three layers simulates a smaller layer spacing as has been pointed out by Laramore et al. [20].

Possibly this effect is more important on a (110) face with small interlayer distances than on the other low index planes of an fcc crystal. Assuming a potential difference of 3 eV between the first and the second layer spacing, and considering the angle and energy range of the measurements, a simulated contraction of no more than 1.5% is found. As this effect depends on the angle of incidence and on the energy as well, it is in principle possible to eliminate this error, but this is not called for in this investigation.

Acknowledgement

Financial support by the Deutsche Forschungsgemeinschaft through SFB 128 is gratefully acknowledged.

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