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DETERMINATION OF DOMAIN DISTRIBUTION BY ANALYSIS OF LEED BEAM PROFILES.

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Abstract

Angular profiles of LEED beams from Au(110)-(1x2) have been measured and analyzed with respect to shape, half-widths and energy dependence of half-widths. Beam broadening is mainly caused by steps. The distribution of terrace widths has been determined, analyzing the shape of the profiles which have been found to be well described by a Cauchy function. This profile is caused by an exponential decrease of domain size probabilities.

1. Introduction

Imperfections in the surface registry, such as statistically distributed domains or steps, cause broadening or splitting of the LEED beams. The average number of defects can be obtained from the half-widths of the angular profiles whereas the information about the distribution of defects is contained in the shape of the profile. In a first approximation the angular profile - after deconvolution with the instrumental function - is given by the Fourier transform of the correlation function. A Gaussian-like distribution of domain sizes causes satellite reflections or splitting of the beams still at rather broad distributions [1]. As Henzler [2] has shown, such splitting disappears and a continuously broadened beam with a Gaussian shape appears at asymmetric distributions of domain sizes where still a preference for a certain domain size exists but short domains are strongly suppressed. A different type of distribution is given by an exponential decrease of domain size probabilities where the shortest domain has the maximum probability. Such a distribution leads to a Cauchy function in the beam profiles and is preferably described by continuing probabilities rather than domain sizes, that means, the distribution is ruled by the probability that one step or domain boundary is followed by another at the next possible lattice place [3]. The physical process producing this distribution is different from that one which causes a Gaussian shape of the profile.

2. Experimental Results

An Au(110) surface has been prepared by spark erosion and electrochemical polishing [4]. After ion bombardment and annealing the surface shows a (1x2) superstructure with slight diffuseness of the diffraction spots in $[001]^*$. Measurements were performed with a Faraday cup with an entrance slit of 0.45x4 mm corresponding to an aperture of $0.44^\circ \times 3.78^\circ$. Angular profiles of (0k) reflections, integer and half order beams, have been measured parallel to $[001]^*$ at energies between 20 and 220 eV at angles of incident $\vartheta = 75^\circ$ and 90°, and of the (h0) reflections in the perpendicular direction $[\bar{1}10]^*$ at the same energies and angles of incidence.

The instrumental function has been determined in a way described by Wang and Lagally [5] from the minima of the half-widths of the (00) beam in $[\bar{1}10]^*$, assuming a Gaussian function of the primary beam convoluted with the Faraday cup slit function.

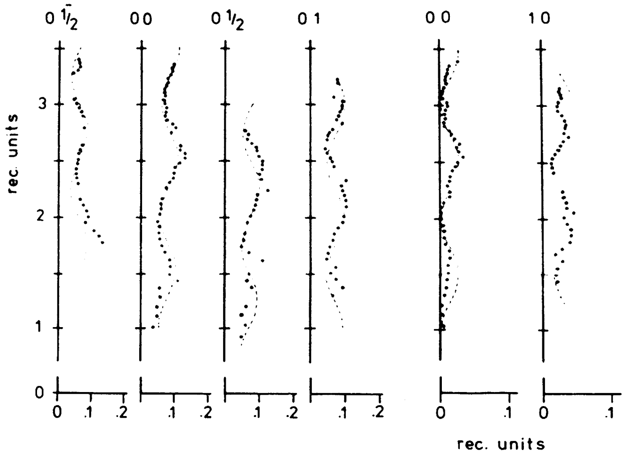

Fig. 1 Half-widths of different beams as a function of the scattering vector, measured in two lattice directions [001] and $[\bar{1}10]$. The dashed lines indicate the theoretical function. Reciprocal units of the bulk lattice are used.

3. Analysis of Profiles

Deconvolution of narrow profiles directly by Fourier transform causes numerical problems which are overcome by a fit procedure in which a theoretical function is convoluted with the instrumental function and compared with the measured profiles. In all cases best fit has been achieved with a Cauchy function as theoretical profile.

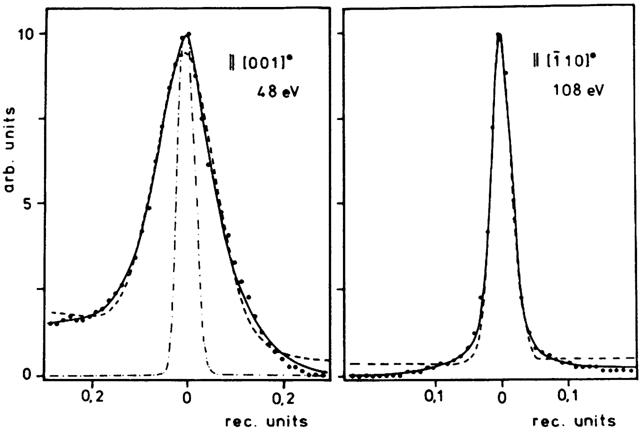

Fig. 2 Angular beam profiles in $[001]^*$ and $[\bar{1}10]^*$. In both directions the profiles are fairly well represented by Cauchy functions.
Solid line:
Cauchy function
dashed line:
Gauss function
full dots:
measurement
The thin dashed line is the instrumental function

It should be mentioned that the information about the correlation function is contained in the profile wings, whereas the half-widths can be determined nearly as well by use of a Gaussian function.

4. Discussion

The energy dependence of the peak widths indicates a stepped surface structure. The integer order beams broaden alternately as can be seen in Fig. 1, and the superstructure beams broaden and sharpen in the same way but are shifted by a quarter of the period. This behaviour is produced by steps which are displaced by a quarter of the superstructure lattice spacing. The step height corresponds approximately to the bulk value of 1.442 Å. A more precise determination of the step height seems difficult because of the uncertainties in the measurements.

All observations are consistent with the missing row model distorted by steps. Of course, profile analysis is not suited for structure determination, but any other structure model must permit the existence of terraces shifted parallel and normal by a quarter of a superlattice spacing and a bulk layer spacing, respectively, as shown in Fig. 3. The existence of antiphase boundaries produced by an occurrence of the bulk lattice spacing can be widely excluded since for this model the integer order beams remain sharp and the half order beams are diffuse, independent of energy.

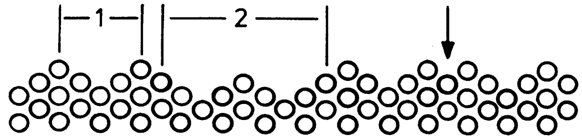

Fig. 3 Two types of lattice faults in the missing row model. The arrow indicates an antiphase boundary (see text for explanation). Terrace widths are related to the superstructure spacing.

A formerly discussed model [6] in which both types of lattice faults have been assumed to occur with equal probability does not produce a sufficient variation of the half-widths of the superstructure beams. We therefore conclude that mainly steps occur at the surface. The existence of other types of faults cannot be excluded completely since the reflections do not get perfectly sharp at any energy in $[001]^*$.

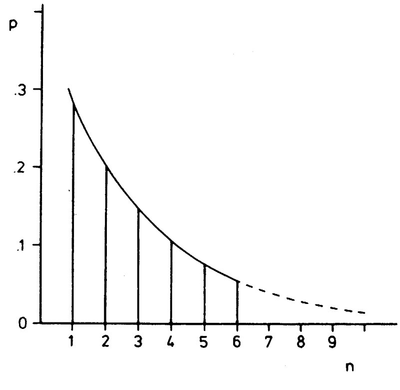

Fig. 4 Distribution of terrace widths. Unit is a superlattice spacing.

This effect could also be a consequence of multiple scattering processes. The distribution of terrace widths follows from the "Cauchy" shape of the profiles. The probability of finding a domain with a single lattice spacing is determined from the maxima of the half-widths shown in Fig. 1.

The average terrace widths are 3-4 superlattice spacings (25-35 Å) in [001] and 25-35 lattice spacings (70-100 Å) in [$\bar{1}$10].

The main uncertainty in the analysis of half-widths and profile shapes is due to the errors made in the determination of the instrumental function. A further limitation arises from the fact that contributions from thermal diffuse scattering to the profile cannot be resolved.

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