Diffraction and focusing effects in the elastic scattering of electrons from Cu(001)

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We have measured polar-intensity plots (PIP's) of the elastic reflection of electrons from Cu(001) in the energy range 200–1500 eV. At low energies, the PIP's present sharp peaks due to low-energy electron diffraction. For $E > 500$ eV, strong peaks appear at the angles corresponding to the main crystallographic axes. We interpret this as being due to the focusing effect that occurs in Auger and x-ray photoelectron diffraction. The importance of this finding is that both the reciprocal and the real (direct) lattices can be explored in the same experiment by simply varying the energy of the electrons.

The phenomenon of electron diffraction is bound up with the development of quantum mechanics. In the context of surface physics, low-energy electron diffraction (LEED) and, more recently, Auger electron diffraction (AED) and x-ray photoelectron diffraction (XPD) have been used for the determination of surface structures. In LEED experiments a monochromatic beam of electrons impinging on the surface is coherently dispersed by the ion cores; the constructive interference which occurs along directions connected to the reciprocal lattice of the surface allows an easy determination of the symmetry and size of the unit surface cell; the content of this cell and the interlayer spacing can be extracted from the diffraction intensities. A loss of coherence in the scattering, due to thermal vibration of the ion cores, limits the electron energy to less than 500 eV in most experiments.

In AED and XPD experiments[1–4] at intermediate electron energies (~ 1 keV), interference effects involving relatively few atoms produce anisotropies in the angular distribution of the emitted electrons. The most prominent of these structures occur at the internuclear directions and have a simple explanation: The outgoing electron is focused along the bond directions by the attractive potentials of the near neighbors of the emitting atom. This forward focusing effect gives rise to maxima in the polar-intensity plot (PIP) of the electron emission at angles connected to the main crystallographic axes and thus to the real lattice.[2–4]

This last point leads us to investigate whether forward focusing plays any role in the elastic scattering of electrons at intermediate energies. The occurrence of such an effect would be of great importance because both the reciprocal and the real lattices could be explored in the same experiment by simply varying the energy of the electrons. We have found that forward focusing indeed occurs in the elastic scattering of electrons, and, furthermore, that it is the dominant effect at electron energies greater than 500 eV. Measuring PIP's of the elastic peak as a function of the electron energy, we have determined the regions of dominance of LEED and forward focusing effects, and the energy dependence of the peaks due to forward focusing.

We have measured the intensity of the elastic reflection of electrons impinging on Cu(001) as a function of the polar angle of emergence along the [010] azimuth and of the energy of the electrons. The experimental geometry is shown in Fig. 1. It is such that during a polar scan the exit direction coincides with several important crystallographic axes but the incident direction does not. We have used a hemispherical electrostatic energy analyzer operated in the constant retard ratio mode with $\Delta E/E = 0.5\%$ and $\pm 6°$ angular resolution. The Cu(001) was oriented and cut by standard methods. It was cleaned by repeated cycles of argon bombardment and annealing at 800 K until a good LEED pattern was obtained and the sulfur concentration (the only contaminant detected by AES) was less than 1%. To isolate the effects due to the crystalline order, we measured also the intensity of the elastic scattering from polycrystalline Cu. The results are presented through the anisotropy factor defined as

$$A = [I(\text{crystal}) - I(\text{polycrystal})]/I(\text{polycrystal}) .$$

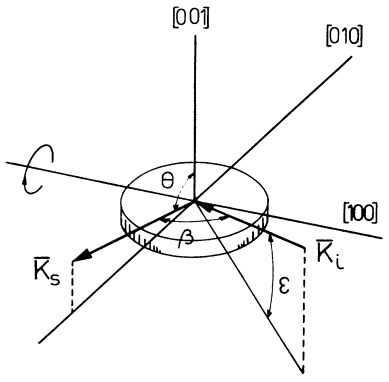

FIG. 1. Schematic illustration of the experimental geometry. When the sample is rotated on the [100] axis, the polar angle of the scattered electrons, θ, and the elevation angle of the incident beam, ϵ, change; the scattering angle $\pi - \beta$ remains constant at 144.35°. For $\theta = 75°$ the elevation angle ϵ is 30°.

The main results of our study are condensed in Fig. 2. A polar-intensity plot of the *LMM* Auger-electron emission ($E=917$ eV) is included for comparison with our results of elastic reflection at intermediate electron energies. This PIP is in good agreement with those reported in the literature.[2,4] Egelhoff was the first to postulate that forward focusing and not electron channeling or Kikuchi effects is responsible for the structures observed in the curve. Single-scattering cluster calculations[5,6] confirmed this for the peaks at 0° and 45° which correspond to emission along the [001] and [011] crystallographic axes. The structure at $\theta \simeq 20°$ has two sources; besides an enhancement due to forward focusing along the [013] axis, there is a first-order interference effect which is expected to be important at this polar angle.[5,6]

The PIP of the elastic peak at 200 eV presents very sharp structures due to LEED effects. It is well known that the coherent dispersion of the incident plane wave by many ion cores produces a set of scattered beams at directions determined by conservation of the energy and the momentum parallel to the surface plus a vector of the reciprocal lattice of the surface. As the sample is rotated, different LEED directions enter the cone of angular acceptance of the energy analyzer; the polar angles at which this is expected to occur are indicated for the PIP's of 200 and 400 eV. At 200 eV two very intense peaks are observed at the polar angles corresponding to the (02) and ($\bar{1}1$) LEED directions (note the important reduction in the intensity scale). The smallness and the absence of the peaks corresponding to the ($\bar{2}0$) and ($\bar{3}\,\bar{1}$) LEED directions are probably related to the occurrence of minima at this energy, 200 eV, in the respective intensity-versus-energy curves.

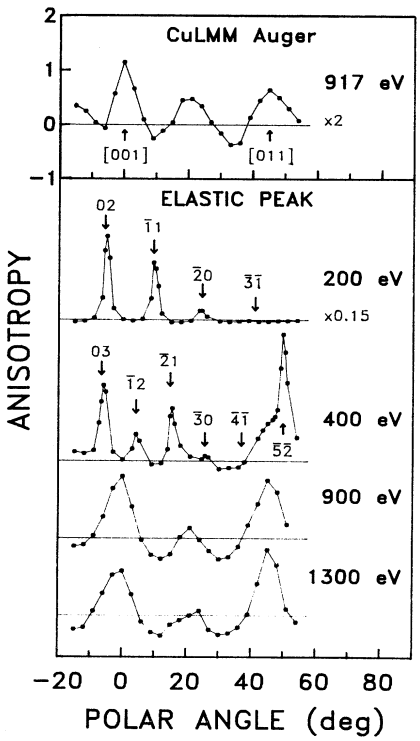

FIG. 2. Polar-intensity plots (PIP's) of the Cu *LMM* Auger peak and the elastic peak at the energies given on the right. The intensities have been normalized to the emission from polycrystalline Cu (see the text); the ordinate scales, shown for the PIP of the Cu *LMM* Auger peak only, are the same for all the PIP's. The arrows indicate emission along crystallographic axes in the PIP of the Cu *LMM* and along the LEED directions in the PIP's of the elastic peak at 200 and 400 eV.

When the electron energy is increased to 400 eV, the agreement between the polar angles connected to LEED directions and the polar angles at which the structures occur is still excellent. Two major effects characteristic of LEED experiments are observed: (i) a contraction of the curve allowing more peaks in the same angular range and (ii) a significant loss of intensity. The first point is a direct consequence of the conservation laws for energy and momentum. The second observation is connected to the loss of coherence in the scattering, an effect which is expected to be important when the wavelength of the electrons becomes comparable with the thermal vibration of the atoms.

At the energy of 900 eV the PIP of the elastic peak has taken the form characteristic of the AED and XPD experiments. Two big peaks at 0° and 45° and a smaller one at $\theta \simeq 20°$ are observed. Note, however, that the anisotropies are a factor of 2 more intense than in the emission of *LMM* Auger electrons. The LEED structures have disappeared as expected on the basis of the loss of coherence discussed above.

Increasing the energy to 1300 eV does not affect the angular position of the two major peaks, only their intensities. This strongly suggests that forward focusing along the [001] and [011] directions is responsible for these anisotropies. The structure at $\theta \simeq 20°$ does change and therefore seems to be connected more to an interference effect and less to enhanced emission along the [013] axis.

To know whether a picture similar to that of AED and XPD is applicable to the case of elastic reflection of electrons at intermediate energies, we have performed a simple single-scattering cluster calculation.[1] In AED and XPD this model considers a superposition of the primary spherical wave and those waves scattered once by the near neighbors of the emitting atom. Interference between the primary and scattered waves gives rise to intensity modulations with the emission direction. The forward focusing effect arises from the strong peaking of the scattering amplitude in the forward direction (bond direction).

To extend this model to our experiment, we have assumed that at intermediate energies the incident electron is backscattered by a single ion core (i.e., we neglect coherence at this stage) and then, in its way to the surface, is scattered into the detector direction by the near neighbors of the backscatterer. The calculation proceeds as in AED and XPD with the only difference that the outgoing spherical wave is $f(\theta)e^{ikr}/r$, where $f(\theta)$ is the plane-wave scattering amplitude.

Figure 3 shows the results of this calculation at $E=900$ eV for a three-atom cluster with the "emitter" in

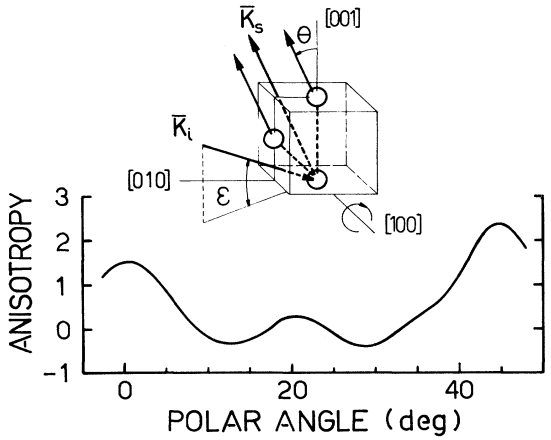

FIG. 3. Result of the calculation for $E=900$ eV with the three-atom cluster shown in the inset. The incident electron is backscattered by an atom in the third layer. Secondary scattering events with atoms in the second and first layers give rise to the anisotropies observed in the experiment.

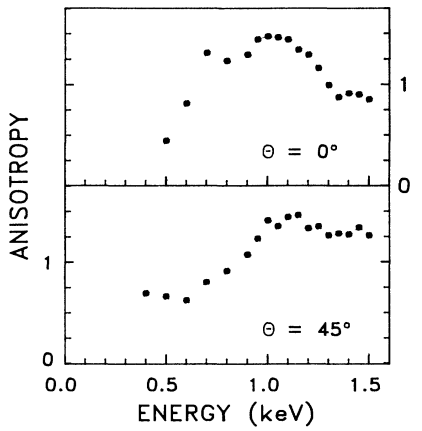

FIG. 4. Intensity of the peaks at 0° and 45° as a function of the electron energy.

the third layer. The excellent qualitative agreement indicates that this simple system contains all the important effects. The peaks at 0° and 45° are due to the focusing effects of the atoms in the [001] and [011] axes, respectively, and the small structure at $\theta\simeq 20°$ is due to constructive interference between the direct wave and the waves scattered in the $\theta\simeq 20°$ direction by the atoms in the first and second layers (this simple calculation does not include the case of forward focusing in the [013] axis). Calculations at other energies show that the angular position of the two major peaks does not change while the small peak changes in position and shape. This is again in general agreement with experiment.

The picture that emerges from the PIP's of Fig. 2 and the results of the calculations is that at low electron energies LEED effects dominate, allowing a determination of the reciprocal lattice vectors. At intermediate electron energies the LEED effects disappear and the phenomenon of forward focusing takes over allowing a determination of real lattice vectors.

The energy dependence of the peaks due to forward focusing effects can also be analyzed with this experiment, and this is shown in Fig. 4. The general behaviors are rather different; although both peaks have a maximum intensity at $E\simeq 1$ keV, the threshold energies and the after maximum behaviors are different. It is evident from Fig. 4 that the peak at 45° starts at much lower energies than the peak at 0°. This is also apparent in the PIP of the elastic peak at 400 eV in Fig. 2, where, besides the LEED peaks, there is a clear shoulder at 45° but no evidence of any enhancement at 0°. It is interesting to note that these energy dependences are in agreement with the observation made by Egelhoff[2] that the PIP of the Cu $2p_{3/2}$ photoelectrons ($E=317$ eV) has the peak at 45° only, whereas the PIP of the *LMM* Auger electrons ($E=917$ eV) has both peaks. This again points to a common origin of the anisotropies in this and in AED and XPD experiments. We have found that the energy dependence of the intensities at 0° and 45° is more complex than the angular dependence at any fixed energy and cannot be accounted for with simple calculations. Larger clusters and/or better approximations are required to fit the curves of Fig. 4. Notice that, similarly to LEED, at intermediate electron energies the PIP's contain easy-to-see information about the surface geometry, whereas valuable atom distances can be extracted from the intensity-versus-energy curves.

As a final and rather picturesque test, we attempted to observe the general behavior contained in Fig. 2 on the screen of a standard LEED optics. The LEED spots could be followed up to 650 eV. At $E\simeq 700$ eV a diffuse luminosity appeared in the directions $\theta\simeq 30°$ along the [110] azimuths, which coincide with the directions of most intense Auger emission according to the intensity mapping of Li and Tonner.[4] This luminosity did not change when the energy was increased up to 1 keV. Therefore, we think that a wealth of information about the real lattice[7] should be easily obtained with the specialized LEED equipment used to measure *I-V* curves.

In conclusion, we have found that when the LEED effects disappear at high energies, the angular distribution of the elastically reflected electrons is not smooth but full of anisotropies due to simple interference effects. Interestingly enough, the most prominent of these anisotropies is due to forward focusing and thus simply related to the main crystallographic axes, making the phenomenon an excellent complement to LEED for the determination of surface structures. The possibility of making the experiment element specific through the analysis of the inelastic scattering (due to core excitations) is presently under investigation.

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[7]See especially Fig. 2 in Ref. 4.