Diffraction of conduction electrons by a copper (012) surface

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The diffraction of conduction electrons by a real copper (012) surface has been observed by means of transverse electron focusing {V. S. Tsoĭ, Pis'ma Zh. Eksp. Teor. Fiz. **19**, 114 (1974) [JETP Lett. **19**, 70 (1974)]; V. S. Tsoĭ and Yu. A. Kolesnichenko, Zh. Eksp. Teor. Fiz. **78**, 2041 (1980) [Sov. Phys. JETP **51**, 1027 (1980)]}.

There are two advantages in using conduction electrons for the structural analysis of surfaces: 1) the low energy of the probing particles, which is on the order of or less than 1 K, and 2) the possibility of an *in situ* study of interior surfaces. A method for determining the translational vectors of a surface by means of electron focusing[1] was worked out in Ref. 2.

The copper sample in the present experiments was cut from a single-crystal bar. The surface of the sample was subjected to the following treatment: polishing with a series of diamond pastes, in which the particle size was progressively reduced from 5 to 0.7 μm; chemical polishing in a solution consisting of 1 part of CH_3COOH, 2 parts of HNO_3, and 1 part of H_3PO_4; annealing in oxygen at 10^{-4} torr and 950 °C for a day; and then a repeated polishing in the same solution. The normal (**n**) to the surface of the

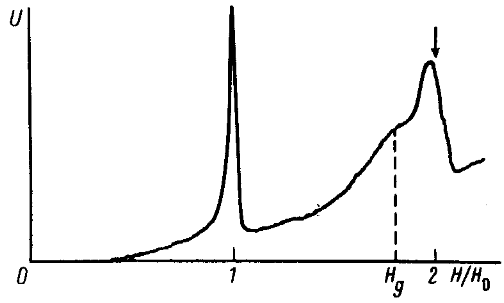

FIG. 1. The dependence $U(H)$. L||[02$\bar{1}$], **H⊥L**.

sample before the polishing coincided within 0.01° with the [012] direction, according to measurements on an x-ray diffractometer.

Two fine tips—the emitter and the collector, made of copper wire—were positioned at the surface of the sample. A current I_e was passed through the emitter, and the voltage (U) on the collector with respect to a peripheral point of the sample was measured as a function of the strength of a magnetic field (H) directed parallel to the surface of the sample and perpendicular to the line of the contacts. The direction of the magnetic field was chosen to cause the trajectories of electrons emitted from the emitter to spiral toward the collector. The contacts were placed along the [02$\bar{1}$] direction; the distance (L) between them was ≈ 0.1 mm.

Figure 1 shows a typical curve of $U(H)$. In a field $H_0 = p_F c/eH$ {p_F is the extreme dimension of the "spherical" part of the Fermi surface of copper along the [012] direction (Fig. 2a)}, we observe a line of electron focusing, formed by electrons that are focused at the collector without reflections at the surface of the sample. A second electron-focusing line, caused by the focusing of the electrons after one specular reflection from the surface, is observed in a field only slightly different from $2H_0$. In addition to these two lines, there is a faint electron-focusing line in a field H_g in the interval $H_0 < H_g < 2H_0$.

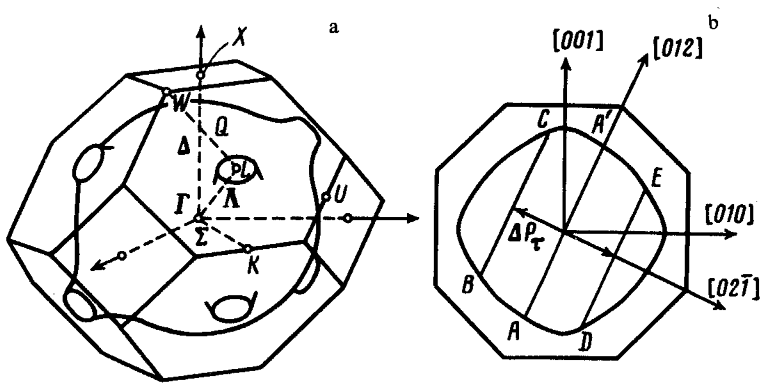

FIG. 2. a—Fermi surface of copper; b—intersection of the Brillouin zone and the Fermi surface of copper with the (100) plane passing through the center of the Brillouin zone.

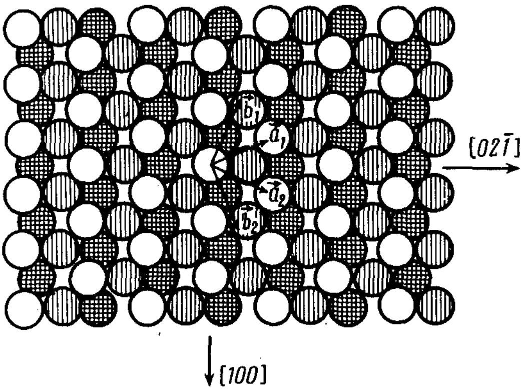

FIG. 3. Structure of the ideal (012) face of an fcc lattice. The atoms lying in different planes perpendicular to the [012] direction are represented by circles shaded in different ways. $\mathbf{a}_1$, $\mathbf{a}_2$—Vectors of the surface lattice; $\mathbf{b}_1$, $\mathbf{b}_2$—the corresponding reciprocal-lattice vectors.

Figure 3 shows the atomic structure of the (012) face of an fcc lattice, such as copper's. The circles shaded in different ways are atoms lying in different planes perpendicular to the [012] direction. Also shown here are the basis vectors of the surface lattice, $\mathbf{a}_1$ and $\mathbf{a}_2$, and the corresponding reciprocal-lattice vectors $\mathbf{b}_1$ and $\mathbf{b}_2$:

$$\mathbf{a}_i\,\mathbf{b}_j = 2\pi\delta_{ij}\,; \quad b_i = 2\pi/a_i \sin\beta\,; \quad b_1 = b_2 = \frac{2\pi}{a}\sqrt{\frac{6}{5}}$$

where β is the angle between the vectors $\mathbf{a}_1$ and $\mathbf{a}_2$, and a is the lattice constant of copper.

Because of the elastic diffraction of electrons at the (012) surface, an electron should remain on the Fermi surface after reflection, but its tangential momentum may change by an amount $m\mathbf{b}_1 + n\mathbf{b}_2$, where m and n are integers. Figure 2b shows the extreme intersection of the Fermi surface of copper with a plane perpendicular [100]. This cross section passes through the center of the Brillouin zone, and for the electrons in this cross section the velocity component along **H** is zero; i.e., the electrons of this cross section move in a plane perpendicular to **H**. It was shown in Ref. 2 that if the tangential momentum component of an electron changes by an amount Δp_τ upon reflection from the surface, an additional electron-focusing line will result. The position of this line along the H scale is determined by the condition that the extreme displacement of electrons along the line of the contacts at a given Δp_τ be equal to the distance between the contacts. Since the vector $\mathbf{b}_1 + \mathbf{b}_2$ is directed along the [02$\bar{1}$] direction (Fig. 3), the electrons of the extreme cross section, whose tangential momentum component changes by an amount $\mathbf{b}_1 + \mathbf{b}_2$ upon reflection, remain in the extreme cross section and continue to move in the previous plane. It is easy to see that the extreme displacement along the line of the contact is that of the electrons in states B and D in Fig. 2b, which lie a distance $(1/2)\Delta \mathbf{p}_\tau = (\mathbf{b}_1 + \mathbf{b}_2)/2$ away from the extreme diameter AA', In a magnetic field, the motion of these electrons in momentum space can be described as follows: from the point B (D) along the extreme cross section to the point C (E), then, because of reflection from the surface, a transition to the point D (B), and a further movement along the extreme cross section to the point E (C). The first electron-focusing line should be observed in a field $H_0 = AA'c/eL$, and the additional line should be observed at $H_g = (BC + DE)c/eL = 2BCc/eL$. For copper we have[3]

$H_g = 1.72H_0$. It can be seen from Fig. 1 that the field at which the additional line is observed agrees satisfactorily with the calculated field, shown by the dashed line in this figure.

We thus see that this feature of electron focusing can be explained on the basis of the diffraction of conduction electrons by the copper (012) face. If this explanation is to be correct, the (012) surface of the real copper sample under the layer of adsorbed atoms and molecules must contain high-quality regions that cause electron diffraction. A high surface quality [of a (011) face] under a layer of adsorbed atoms and molecules has been observed previously for tungsten samples,[4] as was demonstrated by the high probability for the specular reflection of electrons upon normal incidence (0.6); this probability was just as high as that for samples with an atomically clean surface.[5] The (012) face of copper is rather "porous" (Fig. 3), so that the surface of a sample should undergo a terracing during annealing and chemical polishing. It is easy to show that if the surface is a mosaic surface, and the direction of the local normal does not coincide with the direction of the normal to the average surface of the sample, then the electron-focusing lines should shift toward weaker fields at fields that are multiples of each other. The observed shift of the second electron-focusing line (Fig. 1) can be explained in a qualitatively satisfactory way by assuming that there are local terraces with a normal along the [011] direction on the surface of the sample. The case in which the electron-focusing lines shift in fields that are multiples of each other was studied in Ref. 6, where reflection from two faces of the terraces was taken into account.

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