Investigation of the reflection of conduction electrons from the surface of a tungsten sample

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The probability of specular reflection q at normal incidence, for various groups of electrons reflected from the same section of the surface, was measured by the transverse-focusing method. For reflection from the (001) plane, the value of q depends substantially on the position of the electron on the Fermi surface and ranges from 0 to 0.70. All the electron groups are reflected in equal fashion from the (110) plane, $q \approx 0.6$, but if the quality of the surface is artificially deteriorated, then q becomes dependent on the electron wavelength λ. The reflection of electrons of wavelength $\lambda \approx 13$ Å becomes diffuse, and for electrons of wavelength $\lambda = 51$ Å the value of q decreases only to 0.5. It is shown that intervalley scattering processes in specular reflection in tungsten play an inessential role. A possible cause of the diffuse scattering of certain groups of electrons from the (001) plane is taken to be umklapp processes produced in the reflection by singularities of the translational symmetry of the boundary atomic plane (001).

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INTRODUCTION

The possibility of specular reflection of conduction electrons in metals, at either glancing[1-3] or normal[4-7] incidence on the surface, has by now been experimentally established. The conditions under which specular reflection takes place, however, are not clear to this day.

In the investigation of the laws governing the laws of reflection of the conduction electrons from the surface it is necessary to separate two principal aspects: reflection from a perfect surface (i.e., one at thermodynamic equilibrium) and reflection from a surface having random roughness due to imperfections of the crystal, e.g., vacancies, chemical impurities, and others.

In reflection from a perfect surface, an essential role is played by the translational symmetry group of the atomic boundary plane. If it differs from the translational symmetry group of an infinite-crystal atomic plane parallel to the surface, then a reflected electron does not conserve its tangential quasimomentum component p_t.[8] If the aforementioned symmetry groups coincide, then at certain orientations of the reflecting surface the reflection proceeds with conservation of the tangential quasimomentum[8,9] and in the case of a spherical Fermi surface (FS) the conservation of p_t corresponds to the conservation of the tangential component v_t of the velocity with which the charge transport is directly connected, and only in this case are there no size effects in the conductivity.

When electrons are reflected from a surface at sufficiently low temperatures, the electron energy should be conserved, as follows from the single-particle character of the problem,[8] and it is precisely these two conservation laws—of the energy ϵ and of the tangential quasimomentum—which define the concept of specular reflection of a conduction electron. In a metal, in the case of specular reflection of an electron from the surface, the state of the reflected electron may be not single-valued, owing to the multivalley character of the electron spectrum. Situations are possible wherein the conservation laws do not prevent the transfer of an electron from one valley to another in the course of reflection, and in this case the number of reflected states is determined by the number of valleys.

Undoubtedly, a real surface has random roughness that cause the electron reflection to become diffuse (nonconservation of p_t). The question of electron reflection at large incidence angles on a surface with random roughnesses had not been studied to a great degree.[9] It is obvious, however, that in this case the character of the reflection depends essentially on the ratio of the electron wavelength to the dimensions of the roughnesses. In the particular case of glancing electrons or electrons belonging to closed sections of the FS, if the function $\epsilon(\mathbf{p})$ is analytic, the following formula is valid for the probability of specular reflection (for the coefficient q of specular reflection)[8]

$$q=1-2\alpha m v_\perp/\hbar, \tag{1}$$

m is the effective mass, $v_\perp$ is the velocity in the direction normal to the surface, and α is a constant determined by the dimensions of the roughnesses.

By focusing the electrons with a transverse homogeneous magnetic field in multiple fields[5] one determines the change produced in the number of focused electrons by collisions with the sample surface. The decrease in the number of focused electrons after reflection is made possible, in particular, by the diffuse character of the reflection of the electrons by the sample surface, and by the multivalley character of the electron spectrum in the case of specular reflection. Figure 1 shows schematically the possible situation. The Fermi surface (Fig. 1a) consists of three valleys I–III, two electron valleys (I, II) and one hole valley (III). Let the focused electrons traveling from the emitter (point A) be located on the Fermi surface in the vicinity of the point A'. The direction of the normal $\mathbf{n}$ to the surface is shown in the figure. The magnetic field $\mathbf{H}$ is perpendicular to the plane of the drawing. When

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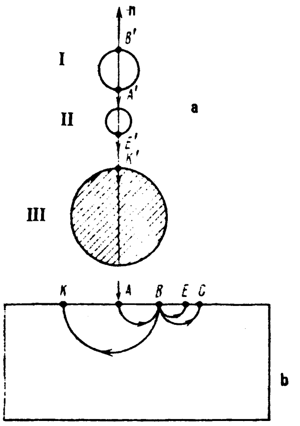

FIG. 1.

the focused electrons collide with the surface they are on the Fermi surface in the vicinity of the point B'. After specular reflection from the surface, the focused electrons can land in the vicinity of the points A', E', K' on the Fermi surface, in which case they will be focused in coordinate space in the points C, E, and K, respectively. Obviously, the processes of scattering at the points E' and K' on the Fermi surface should lead to a decrease of the second electron-focusing line when the collector is placed at the point C and to the appearance of additional electron-focusing lines at a given value of H and when the collector is placed at the points E and K, all of which can be observed in experiment.

The purpose of the present study was to carry out a comparative investigation, with the aid of electron focusing, of the character of reflection from one and the same section of the surface, of various groups of conduction electrons in tungsten at normal incidence; the groups had different momenta (different de Broglie wavelengths) and different topological possibilities of intervalley specular-scattering processes, depending on their positions on the Fermi surface and on the orientation of the reflecting plane. At the same time, recognizing the great possibilities afforded by electron focusing as a research method,[5, 10-12] the observation of electron focusing of electrons in a metal with high carrier density and with a complex Fermi surface is of independent interest.

EXPERIMENT

To observe the electron focusing we used the same experimental setup as before.[5] Two needle points, an emitter and collector, were mounted on the surface of a single-crystal tungsten sample. Current was passed through the emittor, and the voltage between the collector and the peripheral point of the sample was measured as a function of the magnetic field H situated in the plane of the sample and directed perpendicular to the emitter–collector line. The construction of the measuring head for the mounting of the sample and the placement of the contacts is described in [13]. The measurements were made in alternating current at 20 Hz and $T = 1.7$ K, and the sensitivity of the measuring circuit was $\sim 10^{-10}$ V.

We used in the experiments plane-parallel single crystal tungsten planes 1–2 mm thick, with two crystallographic orientations: 1) $\mathbf{n} \perp (110)$ and 2) $\mathbf{n} \perp (001)$; $\mathbf{n}$ is the normal to the surface of the plate. The plates were cut with an electric-spark lathe from an ingot with a resistance ratio $\rho_{room}/\rho_{4.2\,K} = 70\,000$, ground mechanically, and then etched and polished in a KOH solution to which glycerine was added. The electrolytic treatment removed a metal layer ~0.2 mm thick. The crystallographic orientation of the sample was determined by x-ray diffraction.

The needle points were made of tungsten wire of 0.1 mm diam. A series of measurements was made with copper points, and no effect of the point material on the measurement results was noted. The instant when the point touched the sample was determined by the onset of current in the circuit of a battery with one terminal connected to the needle point and the other, through a ballast resistor, to the sample. When the needle points were mounted it was noted that a region with surface defects was produced around the point. The dimension of the region is determined by the values of the battery voltage and of the ballast resistor. A situation, useful in some cases, could be realized when only midway between the contacts was a small section of perfect surface, in which case only the first two electron-focusing lines were observed in practice. In all our experiments the distance L between the contacts did not exceed 0.1 mm.

RESULTS

Singularities of the electron focusing in tungsten. A model of the Fermi surface of tungsten is shown in Fig. 2. The electron part of the surface—the "jack"—has a near-octahedral shape, with convex spherical sections S (spheroids) located on the corners of the octahedron. The hole part of the Fermi surface consists of an "octahedron" H and "ellipsoids" N. The dimensions of the Fermi surface were determined with the aid of the de Haas–van Alphen[14, 15] and the Gantmakher[16] effects.

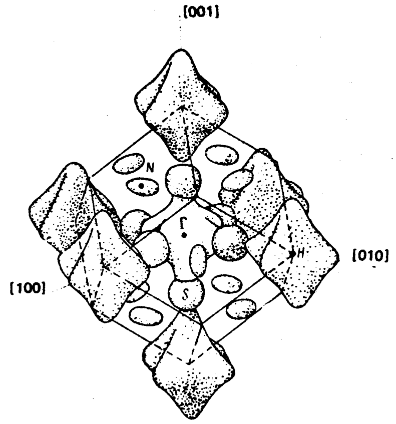

FIG. 2. Model of Fermi surface of tungsten.

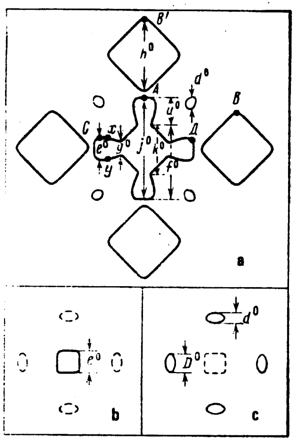

FIG. 3. Intersection of the Fermi surface of tungsten with a plane parallel to (100); $\mathbf{n}\perp(001)$: a—intersection with plane passing through the center of the Brillouin zone; b—extremal section of spheroid; c—extremal section of ellipsoids.

In measurements on the samples with $\mathbf{n}\perp(001)$ the magnetic field was directed along [100] and [110], and in the case of the samples with $\mathbf{n}\perp(110)$ it was directed along [001], [1$\bar{1}$0], and [1$\bar{1}$2]. Figures 3 and 4 show the external sections (solid lines), perpendicular to H, of the Fermi surface of tungsten and the sections of the neighboring sections of the Fermi surface (dashed lines) for some experimental situations. According to the electron-focusing theory,[10] the singularities in $U(H)$ (the electron-focusing line) appear not only in the presence of extremal diameters of the central sections of the Fermi surface at a specified experimental geometry, but also in the presence of dimensions of the type k^0 and xy (Fig. 3a), where x and y are inflection points. It is obvious that the singularity of $U(H)$ should also arise in the presence of dimensions of the type a^0 (Fig. 3a) and is connected with the truncation of the electrons of the spheroids—trajectory-chord dimension corresponding to the dimension a^0 becomes smaller with increasing H than the distance between the contacts, and the electrons of the spheroid cannot reach the collector

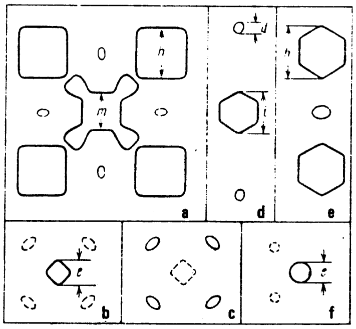

FIG. 4. Intersection of Fermi surface of tungsten (for the case $\mathbf{n}\perp(110)$) with a plane parallel to (001): a—intersection with plane parallel through the center of the Brillouin zone; b—extremal section of spheroid; c—extremal sections of ellipsoids. Intersection with plane parallel to (1$\bar{1}$2): d—intersection with plane passing through the center of the Brillouin zone; e—intersection with plane passing through center of octahedron; f—extremal section of spheroid.

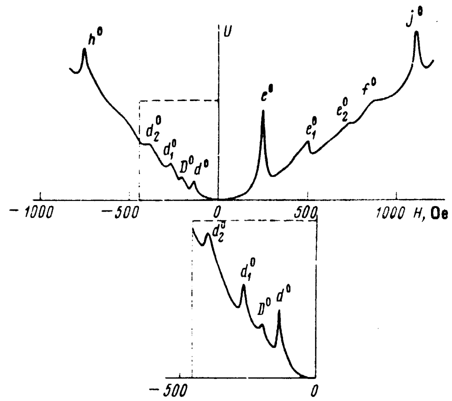

FIG. 5. Electron focusing lines in sample with $\mathbf{n}\perp(001)$ and $\mathbf{H}\parallel[100]$.

from the emitter without colliding with the surface. An interesting circumstance[10] is that the shape of the electron-focusing line is determined by the type of the extremal diameter. In the case of a maximal (minimal) diameter the electron-focusing line has an asymmetric form and a steep wing on the side of the stronger (weaker) fields. When the electron-focusing line is due to a chord joining inflection point, it is symmetric.

We observed in the experiments all possible electron-focusing lines of the extremal diameters (Figs. 5–8), with the exception of the orbit with diameter m (Fig. 4a). In Figs. 3–8 the extremal dimensions and the corresponding electron-focusing lines are labeled by the same letters; the symbol 0 designates the electron focusing line observed in the sample with $\mathbf{n}\perp(001)$. We were unable to observe electron-focusing lines due to dimensions of the type k^0, xy, or a^0 (Fig. 3a). In the experimental geometry with $\mathbf{n}\perp(001)$ and $\mathbf{H}\parallel[100]$ we observed f^0 line (Fig. 5), whose position in the H scale corresponds to the f^0 dimension (Fig. 3a).

The amplitudes of the electron-focusing lines j^0 and h^0 at $\mathbf{H}\parallel[100]$ are extremely sensitive to the accuracy of the setting of the contacts along the [010] directions, and these lines are observed only at an angle interval ±5°, whereas the lines d^0, e^0, i, and e are observed in a wide angle interval ~25°. If the contacts are not accurately mounted, a splitting of some electron-focusing lines is observed.

Reflection of carriers from perfect planes (001) and

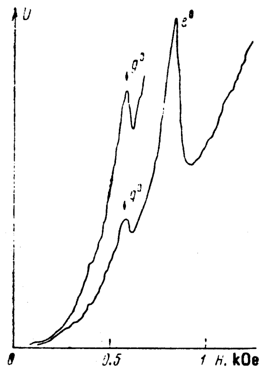

FIG. 6. Line g^0, corresponding to the orbit passing over the neck of the electron jack; $\mathbf{n}\perp(001)$, $\mathbf{H}\parallel[100]$.

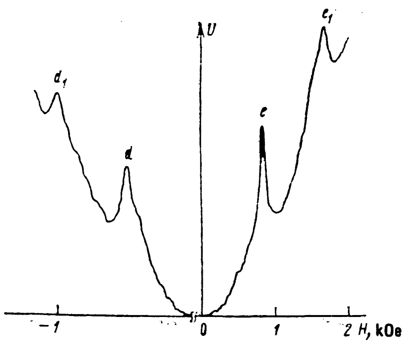

FIG. 7. Electron focusing lines from the spheroid ($H > 0$) and ellipsoid ($H < 0$); n ⊥ (110), H ∥ [001].

TABLE I.

λ, Å	$q_{perfect}$	q_{rough}	Part of Fermi surface
	Plane	(110)	
10.5	0.6±0.1	0	hole "octahedron"
13.5	0.6±0.1	0	electron "jack"
23	0.6±0.1	0.28±0.05	electron "spheroid"
51	0.6±0.1	0.5±0.05	hole "ellipsoid"
	Plane	(001)	
5.7	0		electron "jack"
8.2	0		hole "octahedron"
26	0.25±0.05		electron "spheroid"
50	0.7±0.1		hole "ellipsoid"

(110). When electrons and holes are reflected from the (001) plane there is a substantial difference in the character of the reflection of carrier groups from different sections of the Fermi surface, as is clearly seen in Fig. 5. The specular-reflection coefficients for specular reflection q for normal incidence on the boundary, determined from the ratio of the amplitudes of the electron-focusing lines[5] for different groups of electrons, are listed in the Table I. The most specularly reflected are carriers belonging to the hole ellipsoids: $q \approx 0.70$ (Fig. 5). The coefficient of the specular reflection of the spheroids is much smaller (the same figure): $q \approx 0.25$. We emphasize that these carrier groups are reflected from the very same section of the sample surface.

Carriers from the central sections of the jack (Fig. 0) and the octahedron are reflected diffusely: $q < 0.05$ (there is no second electron-focusing line). The lines of Fig. 9, in contrast to Fig. 5, were drawn for H ∥ [110], inasmuch as in the latter case the j^0 and h^0 line intensities are much higher than in the case H ∥ [100]. The apparent reason is that at H ∥ [100] the extremal orbits with diameters j^0 and h^0 pass along the edges of the jack and octahedron, respectively. To observe the j^0 and h^0 lines in this geometry it would be necessary to pass an appreciable current (~400 mA) through the emitter, and could lead in a strong magnetic field (~2 kOe) to an uncontrollable displacement of the tungsten needle (emitter) under the influence of the ponederomotive force.

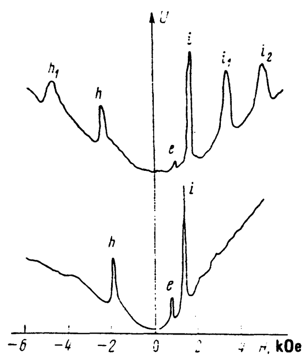

FIG. 8. Electron focusing lines for the jack and the spheroid ($H > 0$) and the octahedron ($H < 0$). Upper curve—perfect surface, lower—artificially damaged surface; n ⊥ (110), H ∥ [1$\bar{1}$2].

There is practically no difference in the character of the reflection of various carrier groups from the (110) plane. The electrons and holes are reflected with the same degree of specularity, $q \approx 0.6$ (Figs. 7,8 upper curves).

Reflection from rough surface. It was noted earlier that deterioration of the quality of the surface [the (110) face] by electrolytic etching did not decrease q by more than 50%. The defects produced in the surface when the contacts are mounted by the procedure described above led to a more substantial suppression of the specularity. By varying the voltage and the ballast resistor it was possible to vary the degree of specularity of the reflection. It is important to note that the produced surface roughness affected differently the character of reflection of different carrier groups. The table lists for comparison the specularity coefficients for different carrier groups from a perfect surface [the (110) plane] and from a surface with defects due to mounting the contacts at a voltage ~200 V, a ballast resistance ~1 kΩ, and $L \approx 0.1$ mm. It is seen from the table that, owing to the defects produced on the surface, the jack and octahedron carriers started to be reflected diffusely (there is no second electron focusing line, Fig. 8, lower curve), whereas the coefficient of the specular reflection for the ellipsoid holes decreased only from 0.6 to 0.5.

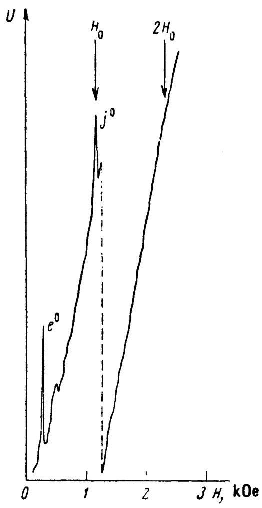

FIG. 9. Electron focusing line from spheroid and jack, n ⊥ (001), H ∥ [110].

DISCUSSION

The experiments have shown that observation of electron focusing in a metal with high carrier density and with a complicated Fermi surface is a problem that can be readily solved, and consequently electron focusing, as a physical method, can be used to investigate a large group of metals. The relative intensity of different electron-focusing lines is explained within the framework of the geometric model of the electron focusing[11,13] and is determined by the number of focused effective electrons. The shape of the electron-focusing line in the case when the extremal section of the Fermi surface has a maximum diameter agrees qualitatively with that calculated by the theory of Korzh[10] and by the geometrical model of the electron focusing.[11,13] The fact that we succeeded in observing a line due to the extremal diameter j^0 ($\mathbf{n}\perp(001)$ but were unable to observe a line due to the extremal diameter m (the same orbit in momentum space, but for the case $\mathbf{n}\perp(110)$), is apparently due to the small electron mean free path l_0 in our samples.

The point is that the number of electrons leaving the emitter and reaching the collector is proportional to $\exp(-l/l_0)$ (l is the path length of the focused electron), and for the orbit with diameter m the value of l is $j^0/m \approx 2.4$ times larger than for the orbit with diameter j^0, and accordingly the intensity of the m line should be smaller by one order than that of the j^0 line, owing to the difference in l. No singularity in the form of the line could be established in the case of the minimal diameter. The electron-focusing lines connected with non-extremal dimensions of the extremal sections of the Fermi surface, if they exist at all, have an intensity much lower than the intensity of the lines in the case of extremal diameters, and it was impossible to observe them. A possible exception is the f^0 line (Fig. 5), which can be connected with the dimension f^0 of the section (Fig. 3a). The absence in this case of a line connected with the dimension a^0 (Fig. 3a) can be attributed to superposition of this line with the e^0 line from the spheroid. The dimensions of the chord and of the diameter are respectively 5.4×10^{-7} and 5.2×10^{-7} cm.

The experimentally observed difference in the reflection from one and the same section of a rough surface of different groups of electrons normally incident on the surface is due to the difference of their de Broglie wavelengths λ.

If the experimental $q(\lambda)$ dependence is described with the aid of formula (1) or with the aid of an approximate formula obtained for a plane electromagnetic wave normally incident on a rough surface[17]

$$q=\exp(-16\pi^3\eta^2/\lambda^2) \quad (2)$$

(η is the mean squared height of the surface roughness), it is impossible to choose the parameter α [for formula (1)] or η [for formula (2)] such that the experimental point fit, within the limits of experimental error, on the $q(\lambda)$ curve drawn in accordance with these formulas. Plots of $q(\lambda)$ [formulas (1) and (2)] that agree qualitatively with the experimental points are shown in Fig. 10. The values of the parameters η and α (α is of the order of the roughness dimension) for these curves are respectively 1.4×10^{-8} and 1.3×10^{-8} cm.

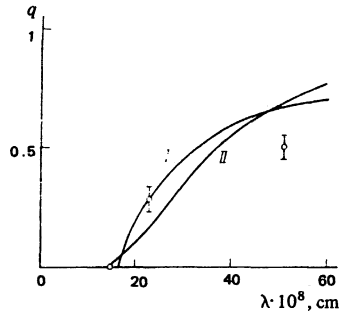

FIG. 10. Extremal points (O) and theoretical plots of $q(\lambda)$. Curves I and II were calculated in accordance with formulas (1) and (2).

Particular interest attaches to the difference in the character of reflection of carriers normally incident on a perfect (001) or (110) surface.[7] Panchenko *et al.*[18] have previously observed, with the aid of the static skin effect, a difference between the reflection of the carriers from automically pure (001) and (110) planes and have proposed to attribute this phenomenon to intervalley scattering processes. The results of the present work show, however, that the role of umklapp processes with conservation of the tangential component of the quasimomenta (vertical U processes) is negligible. This is evidenced by the fact that the carriers from the ellipsoids (orbit d, Fig. 4d), spheroids (orbit e, Fig. 4b), the jack (orbit i, Fig. 4d) all have the same specular-reflection coefficient. It is obvious that the investigated situations are substantially different from the point of view of the topological possibilities of intervalley scattering processes. Favoring this point of view is the fact that the carriers of the ellipsoids (orbit d^0) are reflected from the (001) plane specularly, and from the spheroids (orbit e^0) much more diffusely, although the possibility of intervalley scattering processes are practically the same in these cases (see Fig. 3).

It is not excluded that the difference in the character of the carrier reflection from the planes (001) and (110) is due to the different structure of the roughnesses, and the difference in the character of the reflection of the different groups of carriers from the (001) plane is due to the difference of their wavelengths λ. We wish, however, to point to one possible cause of the difference in the character of the reflection from perfect (001) and (110) planes.

The point is that the law of conservation of the tangential quasimomentum is the consequence of the translational symmetry of a semi-infinite crystal in the crystal plane.[8,9] It is possible to introduce a surface lattice and by applying the Bloch theorem determine the possible states of the reflected electron, taking into account at the same time the energy conservation law.[8,9] The important fact is, however, that the basis reciprocal vectors of the surface lattice can be different from the basis reciprocal vectors lying in the same

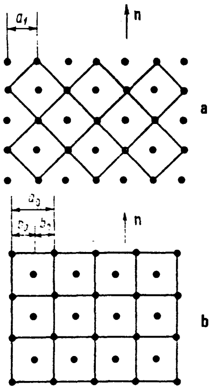

FIG. 11. Projection of body-centered cubic lattice of tungsten on the (001) plane: a) $\mathbf{n} \perp (110)$; b) $\mathbf{n} \perp (100)$.

plane of the infinite lattice. And since the conservation of the tangential quasimomentum is obviously satisfied accurate to the vectors of the reciprocal surface lattice, U-processes are possible wherein the tangential component of the quasimomentum is changed by an amount equal to the vector of the reciprocal surface lattice (horizontal U processes). In our case, when the basis vectors of the surface lattice do not coincide with the basis vectors of the same plane of the infinite lattice, the state to which the electron goes over as a result of the horizontal U process is not equivalent to the initial state.[1)]

The foregoing considerations are illustrated in Fig. 11. Obviously, for the boundary plane (110) the vector of the reciprocal surface lattice in the $[1\bar{1}0]$ direction and the vector of the reciprocal lattice vector of the infinite crystal coincide (Fig. 11a). In this case the horizontal U processes do not change the state of the electron. In the case of the (100) face (Fig. 11b) the distances between the neighboring atoms on the surface a_0 is twice as large than the distance between the neighboring atomic planes b_0. Thus, the reciprocal lattice of the surface $1/a_0$ in the [010] direction is half as large as the reciprocal-lattice vector of an infinite crystal in the same direction. Therefore the electron from state A, for example, lands after a horizontal U process in state B (Fig. 3a). However, it can land in the equivalent state B' with the aid of a vertical U process. Great interest attaches to the possibility that a focused electron of a spheroid (state C; Fig. 3a) will hop over to the point D and by the same token decrease the number of focused electrons after reflection from the surface, hence to decrease q.

In a recent paper, Felter *et al.*[19] used slow-electron diffraction to observe a surface phase transition that leads to doubling of the periods of the surface layer of the atoms of the (001) face of tungsten at ~160 K. The authors note that the presence of adsorbed atoms (which are undoubtedly present also on the surfaces of our samples) hinder the transition. But if such a phase transition does take place, the reciprocal vectors of the surface lattice decrease by one half, and additional possibilities of horizontal U processes appear.

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