# Determination of the amplitude of surface-atom oscillations by field ion microscopy

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A method is proposed for determining the amplitude of the oscillations of surface atoms on jogs of close-packed planes. The amplitude of the oscillations is calculated from the rate of low-temperature evaporation of the metals in strong electric fields; this rate is measured with the aid of a field ion microscope.

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To study the oscillations of atoms on the surfaces of solids it is customary to use crystal physical characteristics that depend directly on the amplitude of the deviation of the surface atoms from equilibrium position. The dynamics of the surface atoms was quantitatively investigated by the method of diffraction of slow electrons[1,2] and of the Mössbauer effect on resonant nuclei located in the surface layer of the crystal.[3] In these experiments and in most theoretical studies[4–6] they investigated oscillations of atoms located in close-packed planes.

We show in this paper that the field ion microscopy method makes it possible to determine the oscillation amplitudes of atoms located on jogs of close-packs atomic faces. Such data are of particular interest, since the oscillations of these atoms determine to a considerable degree the kinetics of the evaporation and growth of crystals, adsorption, corrosion, and many other phenomena on crystal surfaces.

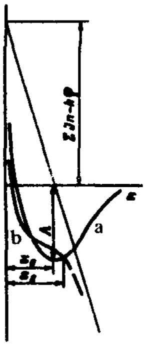

FIG. 1. Diagram of potential energy of a surface atom (a) or ion (b) in an electric field.

The amplitude of surface-atom oscillations on a fracture is determined in the present paper on the basis of field-ion-microscopy data on the rate of the low-temperature evaporation of the metal in strong electric fields.

The rate of evaporation of the atoms is monitored by the height $Q_n$ of the potential barrier (Fig. 1), which is equal to the difference between the energies of the surface atom in the equilibrium position $x_0$ and at the point $x_c$ where the atomic (*a*) and ionic (*b*) potential-energy curves intersect[7]:

$$Q_n = \Lambda + J_n - n\phi - (n^2 l^2/4x_c) - nEx_c, \tag{1}$$

where $\Lambda$ is the heat of sublimation, $J_n$ is the potential of $n$-fold ionization, $\phi$ is the work function of the electron, $e$ is the electron charge, and $E$ is the electric field intensity.

At temperatures below the Debye temperature we have in the usual case $Q_n \ll \Lambda$, and consequently the point of intersection of the atomic and ionic curves lies near the bottom of the well ($x_c \approx x_0$). We can therefore neglect the anharmonicity effects and use for the determination of the evaporation rate $k_e$ the normal distribution[8]

$$k_e(E) = k_0 \exp\left\{-\frac{[x_c(E) - x_0]^2}{2 < x^2 >}\right\}, \tag{2}$$

where $\langle x^2\rangle$ is the mean square of the atom oscillation amplitude component normal to the surface and $k_0$ is the evaporation constant.

At $x \geq x_c$ the ion curve approaches the potential-energy line of an ion in an external field, so that $neEx_c \approx$ const, whence $dx_c/dE = -x_0/E$, and expression (2) can be transformed into

$$< x^2 > = 2\left(\frac{x_0}{E\,(d/dE)\ln k_e}\right)^2 \ln(k_0/k_e). \tag{3}$$

Relation (3) was used to determine $\langle x^2\rangle$ and the Debye temperature of the atoms of single-crystal tungsten 99.95% pure, located on fractures of jogs of {110} planes. Field ion microscopy was used to determine the dependence of the evaporation rate $k_e$, in the interval $10^{-3}$–$10^{-4}$ at. layers/sec at 78°, on the electric field intensity. Evaporation rates higher than one atomic layer per second were reached by connecting the samples to high-voltage pulse generators with pulse durations 0.5, 20, 200, and 700 μsec; the rates were measured by counting the number of pulses in the time when one atomic layer was evaporated.

As seen from Fig. 2, $\ln k_e$ increases practically linearly with $E$; the sensitivity of the evaporation rate to the field intensity, $(d/dE)\ln k_e$, is equal to 39.2 Å/V.

Substituting in (3) $k_e = 1$ at. layer/sec, $E_0 = 5.8$ V/Å, $x_0 = 1.3$ Å, and $k_0 = 5 \times 10^{10}$,[7] we obtain $\sqrt{\langle x^2\rangle} = 0.041$ Å.

It is known that below the Debye temperature there is observed a deviation from the linear dependence of the oscillation amplitude on the temperature $T$; the oscillation amplitude turns out to be proportional here to a certain "effective" temperature[9] $T_e$ such that the difference $T_e - T$ is proportional to the contribution made to $\langle x^2\rangle$ by the zero-point oscillations of the lattice.

The rate of evaporation in an electric field can be represented in the form

$$k_e(E) = k_0 \exp\left[-\frac{Q_n(E)}{k\,T_e(T)}\right]. \tag{4}$$

Substituting the obtained experimental values of $k_e(E)$ in (4) and using the data on the temperature dependence of the "threshold" intensity of the evaporating field, corresponding to an evaporation rate $k_e \approx 10^{-2}$ at. layers/sec,[10] we obtain the function $T_e(T)$ (Fig. 3, curve 1). For comparison, we show a plot of $T_e(T)$ for tungsten surface atoms located inside the {110} plane, as calculated from the deviation of the $\langle x^2\rangle(t)$ plot from a

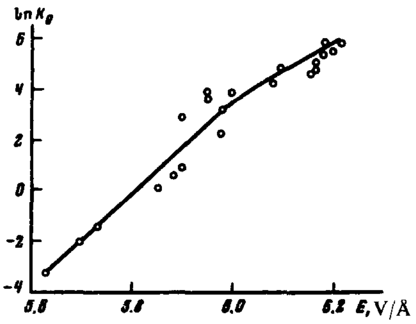

FIG. 2. Dependence of the rate of evaporation of the atoms from the face (110) of tungsten on the field intensity.

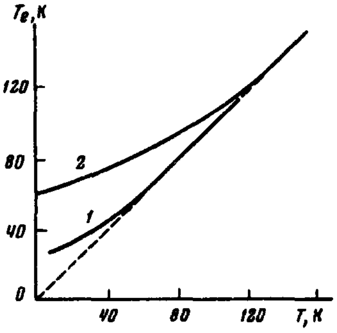

FIG. 3. Temperature dependence of the effective surface temperature on jogs (1) and in the (110) plane (2).

straight line in the low-temperature region. It follows from Fig. 3 that at $T = 78$ °K the contribution of the zero-point oscillations to $\langle x^2 \rangle$ is small ($T_e \approx T$), and consequently, when determining the Debye temperatures for fractures of atomic jogs one can use the high-temperature approximation,[11]

$$\Theta_c^2 = \frac{3\hbar^2 T}{mk \langle x^2 \rangle}, \qquad (5)$$

where $m$ is the mass of the surface atom.

Substitution of the obtained value of $\langle x^2 \rangle$ in (5) yields $\Theta_c = 183$ °K. This is somewhat lower than the Debye temperature $\Theta_s$ for atoms located in the plane ($\Theta_s = 245$ °K[11]). This explains, in particular, why quantum effects begin to influence the amplitudes of the oscillations of atoms on fractures of atomic jogs at relatively low temperatures (see curves 1 and 2, Fig. 3).

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