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SIMULATION OF DENSITY FLUCTUATION OF POTASSIUM ADATOMS ON W (112)

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Abstract - The oscillation part of the effective indirect interaction between potassium adatoms adsorbed on (112) plane of tungsten was used to simulate the dynamics of adsorbed atoms. Simulations of field emission flicker noise have been done using a standard Monte Carlo method. A lattice used in simulation was 18×29 . For three positions of the collector the mean square fluctuations have been computed. Results are in qualitative agreement with the experiment. A $c(2 \times 2)$ structure is created for the low temperature limit.

PROCEDURE

The considered adsorption system is potassium adsorbed on the (112) plane of tungsten. The oscillation part of the effective indirect interaction was used to simulate the dynamics of adsorbed atoms. Because the distances between the adatoms are large, larger than $4.46 \text{ \AA}$, we can assume the interaction energy between the adatoms in its asymptotic form $/1/$

$$V_{as} = A \frac{\cos(2k_F r)}{r^3}, \quad A = \frac{9\pi^2 |W_b(2k_F)|^2}{4k_F^5}, \quad (1)$$

where:

r is the distance between the adatoms, W_b is Fourier transform of a single atom pseudopotential, k_F describes the electron density n :

$$k_F = (3\pi^2 n)^{1/3}, \quad \text{In the above equations atomic units are used.}$$

To estimate A we assume according to Ashcroft $/1/$

$$W_b(2k_F) = \frac{-4 \cos(R_m 2k_F)}{\Omega_0(2k_F)^2}, \quad (2)$$

where for potassium $R_m = 2.13$ and $\Omega_0 = n^{-1}$.

An attempt has been made to simulate concentration fluctuations of potassium atoms on the (112)W for a coverage equal to 0.4. Simulations have been performed on the lattice consisting of 18×29 sites. It gives in a real scale a square of about $80 \times 80 \text{ \AA}^2$.

Fig. 1. The lattice used in simulation. The applied collector positions are seen.

Three collectors of the same dimensions were placed on the surface as shown in Fig. 1. The standard procedure with periodic boundary conditions has been applied for simulation [2]. The atoms were placed randomly on the surface until a coverage equal to 0.4 has been reached. The interaction energies according to E_q (1) have been taken into account assuming that the adatoms can occupy the adsorption sites rather than saddle positions. These energies are presented in Fig. 2.

Fig. 2. Interaction energy versus adatom distance for potassium adatoms on tungsten according to $E_q/1/$.

When the coverage 0.4 has been reached the diffusion run started. For a randomly chosen atom the jump direction was chosen randomly. If the chosen place for the jump was occupied the atom remained at its initial position. If empty, the interaction energy with neighbours was calculated for both initial and intended positions. If the jump did not lead to a higher energetic position the jump occurred with probability $P=1$. In the other case the jump was realized with probability

$P = \exp(-Q/kT)$ where T is the temperature of the system and Q is the difference between the adatom energy V_{as} in intended r_i and initial r_j positions,

$$Q = V_{as}(r_i) - V_{as}(r_j). \quad (3)$$

The existence of "channels" on the (112)W was marked assuming the ratio 3 to 7 of intended jumps in the (110) direction to the (111) direction. The diffusion run was performed until the whole energy of the system was minimal. It means the energy began to fluctuate about its mean value. It was after 300 Monte Carlo steps /MCS/ from a random position of atoms. After that time the measurements began. After each MCS the number of atoms in the collector area was counted. The measurements consisted of about 300 MCS. After that time the mean square number of atoms for each collector was counted.

Fig. 3. a/ Monte Carlo results of mean square fluctuations versus collector positions. b/ the same obtained experimentally [3]. c/ c(2x2) structure obtained for low temperature limit.

In Figure 3 a,b, the simulations results and the comparison of them with experimental data [3] are presented. Figure 3a shows the mean square density fluctuations versus collector position obtained by simulations. Experimental results of mean square fluctuations for $T=400$ K are presented in Fig. 3b. For $T=50$ K the fluctuations were not observed, a c(2x2) structure has been created /Fig. 3c/.

DISCUSSION

For the high temperature limit /Fig. 3a/ the angular dependence of density fluctuations obtained by simulations has a maximum for the (110) direction. It is the case where the interaction energies do not influence the jump decision and the existence of maximum is due to the symmetry of the (112) plane. With decreasing temperature the interaction energies influence the probability of jumping.

Taking $k_F = 1.4 \text{ \AA}^{-1}$, according to [4], we assume that the interaction goes through the electrons of the substrate. The experimental results of Tsong [5], Casanova and Tsong [6], Fink and Ehrlich [7] seem to confirm such assumption. The authors have found the oscillation interaction between the adsorbed atoms for very low coverages.

The formation of clusters at about 500 K indicates that the interaction energies have reasonable values. Approximately good agreement of the maxima and minima of the V_{as} versus r dependence with the adsorption sites is also a result of choosing k_F for tungsten. The decrease of T leads to cluster formation of $c(2 \times 2)$ structure and simultaneously the increase of the mean density fluctuation in the [111] direction is observed. The $c(2 \times 2)$ structure at the low temperature limit was observed as it was expected. For the interaction energy given by Eq.(1) it is energetically favourable.

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