

Let's calculate the modulus of the vector \vec{E}_0 acting along the perpendicular axis to the surface

$$E_0 = E_\theta \cos(\theta) = \frac{d}{4\pi\epsilon_0} \frac{\cos^5(\theta)}{R^3} \left[\frac{3\vec{r}}{|\vec{r}|} - \frac{\vec{d}}{|\vec{d}|} \right] = \frac{d}{4\pi\epsilon_0} \frac{\cos^5 \theta}{R^3} \vec{e}_d (3 \cos \theta + 3 \sin \theta - 1). \quad (3)$$

where \vec{e}_d is a unit vector in the direction of the dipole axis.

Then the projection of the field strength acting from the angle θ to the direction R is equal to

$$E_R = E_0 N(\theta) = \frac{d \vec{e}_d \cos^4 \theta \sin \theta}{2\epsilon_0 R^2 a_0} \times (3 \cos(\theta) + 3 \sin(\theta) - 1). \quad (4)$$

The field strength acting on the ion is calculated by integrating E_R along the angle θ from $-\pi/2$ to $+\pi/2$:

$$E(R) = \int_{-\pi/2}^{\pi/2} E_R \frac{d\theta}{\pi} = \frac{d \cdot 0.5890486}{2\pi\epsilon_0 R^2 a_0}. \quad (5)$$

We get the formula for the dependence of the potential on the distance R from here:

$$\Delta V(R) = - \int_{R_0}^{R_\infty} E(R) dR = \frac{d \cdot 0.5890486}{2\pi\epsilon_0 a_0} \left[\frac{1}{R_\infty} - \frac{1}{R_0} \right]. \quad (6)$$

2. Estimation of the value a_0

It follows from formulas (5) and (6) that the DEL in the model is described by the value $\beta = \Delta x/a_0$, i.e. the ratio of the thickness of the DEL to the average distance between the oriented dipoles. We know from the experimental data [1] that ΔV is estimated at ~ 10 V. Then it follows from formula (6).

$$\beta = \frac{2\pi\epsilon_0 R_0 \Delta V}{0.5890486 \cdot e}. \quad (7)$$

Assuming that $R_0 \approx 5 \text{ \AA}$ and $\Delta x \approx 5 \text{ \AA}$ and the ions repulse from the effective charges of the surface, we obtain that the average distance between the dipoles is $\approx 15 \text{ \AA}$. This is indirectly confirmed by the fact that in experiments [4,5] a SI spectrum is observed which approaches in complexity the spectrum of impact ionization by electrons.

3. Independent confirmation of the existence of a double electric layer on the surface of a semiconductor

Na_xAu_y is its own semiconductor, which follows from the method of its preparation by sputtering of Na atoms

on the surface of gold in high vacuum. The band gap of the semiconductor is $E_g \sim 2.3 \text{ eV}$ with the work function $\phi \sim 4.8 \text{ eV}$, coinciding with the work function of gold. Let's calculate the density of the number of charge carriers in the semiconductor volume at a temperature of $T = 1100 \text{ K}$ using the formula:

$$p = 2 \cdot \left(\frac{m_e k T}{2\pi \hbar^2} \right)^{\frac{3}{2}} \cdot \exp \left(- \frac{E_g}{2kT} \right), \quad (8)$$

where m_e — the mass of the electron, k — Boltzmann constant. Suppose that the distance between charges of the opposite sign is $\Delta x \sim 5 \text{ \AA}$ and $a_0 \sim 50 \text{ \AA}$. Then the volume $V_a = a_0^2 \cdot L$, where $L \sim 100 \text{ \AA}$ (semiconductor thickness) contains no more than $2 \cdot 10^{-4}$ charge carriers. Therefore, the volume of the semiconductor is not involved in the creation of DEL on the surface.

Na atoms are easily ionized on the surface of a semiconductor AuNa since $V - \phi = 5.14 - 4.8 \text{ eV} = 0.34 \text{ eV} > kT \approx 0.1 \text{ eV}$, where V — the ionization potential of Na atoms.

Figure 1 in [6] shows a graph of the dependence of the ion yield Na^+ from the semiconductor surface Na_xAu_y for different temperatures. It is qualitatively different from typical graphs of SI [2]. We obtained a curve for the dependence of ion yield from the surface on temperature by optimizing the curve parameters:

$$\frac{I}{I_0} = \frac{B}{1 + A^{-1} \cdot \exp \left(\frac{V - \phi}{kT} \right)^2} + 1. \quad (9)$$

where I/I_0 is the ion yield in relative units at the following parameter values: $B = 0.664$, $A^{-1} = 5.725 \cdot 10^{-8}$ (Fig. 2). Compare function (9) with the Saha-Langmuir curve describing the ion yield of „classical“, SI. The difference from Saha-Langmuir is:

a) the exponential factor is a quadratic function of $(V - \phi)/kT$,

b) the value of the parameter A , corresponding to the ratio of the number of ionized states of the system to neutral ones, is extremely high.

The analysis shows that the function (9) corresponds to the ionization of two Na atoms on the surface at once. The value A corresponds to the model of repulsive desorption developed and described in section 1 of this paper. The ion yield curve does not contradict the model of ion repulsion Na^+ from DEL oriented dipoles.

4. The model of the occurrence of DEL at the surface

Suppose that under the impact of an external electric field E , the process of charge transfer from Na atoms to Au atoms is actively underway. It is possible to enter dimensionless

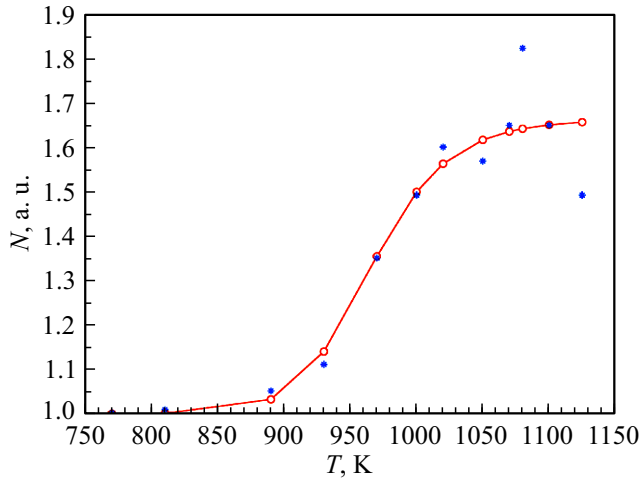


Figure 2. Dependence of the ion yield Na^+ from the surface Na_xAu_y on the substrate temperature. The fitting curve is shown by a continuous red line. The experimental points are shown by blue color.

parameter

$$\left(\frac{\hbar c}{k_B T}\right) \left(\frac{eE}{k_B T}\right) \quad (10)$$

to describe this process. Using the formula (10), we calculate the value E_2 , at which the parameter is equal to one at the experimental temperature $T = 1100$ K, and compare it with the experimental data Fig. 3 [7]. The result is $E_2 \approx 8000$ V/m. The process of restructuring the semiconductor surface is completed at this value of the field and the first broadening of the spectral line Na^+ appears.

Suppose that the Na atoms on the surface of Na_xAu_y can occupy three stable positions:

- 1) The Na atom is located on the surface of the semiconductor above the Au atom,
- 2) The Na atom makes up the upper layer of the semiconductor surface, combines with four Au atoms in the upper layer and one Au atom of the second layer,
- 3) The Na atom is located in the second layer of the semiconductor surface, and the Au atom from the first layer above it is missing.

Desorption of Na atoms from these three locations on the surface results in a broadening of the Na spectral line due to a significant difference of the binding energy of Na to the surface in these three cases.

Assuming that all Na atoms on the surface participate in charge transfer, then the average value of the distance between the dipoles on the surface $a_0 \approx 2a$, where a is the interatomic distance between the planes of the crystal lattice, characterizes the charge transfer process. Dipole DEL with a thickness of a is formed at the semiconductor surface under the action of a weak pulling field E and temperature T , which is in good agreement with the desorption model from section 1. Charge transfer to the internal atomic planes of a semiconductor occurs with an increase of the field E , and the parameter d in the desorption model increases.

Let's try to clarify the physical meaning of the introduced dimensionless parameter (formula (10)). Let's express $\hbar c$ in terms of the fine structure constant α . Multiply and divide by Δx — the distance between charges of different signs of the double electric layer. Then we can easily get an expression

$$\begin{aligned} \left(\frac{\hbar c}{k_B T}\right) \left(\frac{eE}{k_B T}\right) &= \frac{e^2}{4\pi\epsilon_0} \cdot \frac{eE}{(k_B T)^2} \cdot \frac{1}{\alpha} = \frac{e^2}{4\pi\epsilon_0 \Delta x} \\ &\times \frac{e\Delta x E}{(k_B T)^2} \cdot \frac{1}{\alpha} = \frac{e^2}{4\pi\epsilon_0 \Delta x} \cdot \frac{d \cdot E}{(k_B T)^2} \cdot \frac{1}{\alpha}, \end{aligned} \quad (11)$$

where d — dipole moment. It shows that the introduced parameter characterizes a double electric layer on the surface induced by an applied electric field.

The formula (11) shows that DEL plays the role of a point charge acting on the second charge.

And finally, consider the relationship of the charge mobility coefficient with the charge diffusion constant

$$\mu = \frac{eD}{k_B T}. \quad (12)$$

Then

$$\mu E = \frac{eE}{k_B T} \cdot D = v = \frac{a}{\Delta t}. \quad (13)$$

It is possible to estimate the value of D using the following measurements: $\Delta t = 16$ s at $E = 2500$ V/m in Fig. 6 from [1], where $a \approx 5$ Å. We get $D \approx 10^{-15}$ m²/s for $T = 1100$ K.

5. Increase of temperature of desorbed ions

The temperature of desorbed ions can be estimated within the framework of the developed desorption model. Let's consider a desorbable ion on the surface of a semiconductor. The Hamiltonian of this ion has the following form

$$H = \frac{mv^2}{2} + q\Delta V(R). \quad (14)$$

Hence, the ion velocity is easily calculated far from the surface:

$$v = v_0 + \sqrt{\frac{2}{m} \int_0^\infty dx \sqrt{q\Delta V(x)}}, \quad (15)$$

where expression (6) is taken for $\Delta V(R)$. Substituting the parameter values, we estimate the ion temperature at $T \sim 2000 - 3000$ K.

6. Discussion

The symbiosis of the yield of organic ions and Na ions is explained based on the model, since the desorption in the model depends only on the ratio of the values of the surface

potential and the ionization potential of the molecule. The richness of the spectrum of SI organics is also described by our model, since the ion desorption threshold is high enough and all ions with an ionization potential below the threshold are desorbed.

The creation of DEL on the surface is a well-studied phenomenon [8,9]. Surprising is the change of the polarity of the DEL on the surface under the action of a weak pulling field E . It is possible to hypothesize why this is happening. The fact is that Na and Au differ greatly in their electronegativity. Au has the highest electronegativity among metals — 2.84. Na, like other alkali metals, has a low electronegativity ~ 0.7 , so it easily gives away the valence electron to Au. An abnormal polarity DEL is formed on the surface as a result. It should be noted that it was necessary to create conditions of ultra-deep vacuum for implementation of this effect.

Conclusions

The developed model of repulsive ion desorption in SI involves the creation of DEL oriented dipoles on the surface of a specially created semiconductor. Recent studies of the SI of complex organic compounds from the surface Na_xAu_y [4,5] confirms the relevance of studies in this field of surface phenomena. It is desirable to determine the properties of DEL in the future: the dependence on the surface temperature and the magnitude of the pulling field and check the correspondence of formula (10) to the experiment.

Conflict of interest

The author declares that he has no conflict of interest.

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