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QUANTUM STATISTICAL MODELS
IN THE THEORY
OF SUBMONOLAYER COVERAGES

In the present paper, using the method developed in ref. [1] we analyse models that occur for describing the chemisorption of hydrogen-like atoms on crystal substrates of simple metals. This problem is important both from the fundamental and practical points of view as it deepens our understanding of the physical processes on surface in catalysis, hydrolysis and corrosion [2]. Further we shall consider the hard-bond case of hydrogen-like adatoms in the ground state with $(0,0,1)$-plane of a metal surface of a simple cubic symmetry. The jumps of impurities over adsorption centres $\vec{R}_d$ and vibrational degrees of freedom are neglected. The original Hamiltonian of the system considered in this case is

$$H = H_A + H_{\Sigma} + H_{\Sigma A} \quad ,$$

$$H_A = \sum_{j=L}^{M} u(\vec{R}_{d_j}) + \frac{1}{2}\sum_{i\neq j}^{M} v(\vec{R}_{d_i}-\vec{R}_{d_j}) \quad , \quad H_{\Sigma A} = -\sum_{i\,j}^{NM} v(\vec{R}_{d_j}-\vec{x}_i) \quad , \tag{1}$$

$$H_{\Sigma} = \sum_{i=1}^{N} \frac{\hat{P}_i^2}{2m} + \frac{1}{2}\sum_{i\neq j}^{N} v(\vec{x}_i-\vec{x}_j) - \sum_{i=1}^{N} u(\vec{x}_j) \quad .$$

Here H_{Σ} is the Hamiltonian of an electron subsystem, $v(\vec{x}_i-\vec{x}_j)$ is the Coulomb interaction of two charges of the same sign, $u(\vec{x}_j)$ ($u(\vec{R}_{d_j})$) is the interaction of an electron (ion) with a field created by the fixed positive-charged ions of a metal substrate, H_A is the Hamiltonian of an ion subsystem. It has the same structure as H_{Σ} with the exception of a kinetic energy of ions which is neglected, $H_{\Sigma A}$ is the interaction between Σ and A systems. Numbers N and M are total amount of electrons and adatom ions, respectively.

Let us introduce the operator functions of fields $\psi^+, \psi, \phi^+, \phi$ in the form:

$$\psi^+(x) = \sum_{KG} a_{KG}^+ \varphi_{KG}^*(x) + \sum_{\alpha G} b_{\alpha G}^+ N_\alpha \varphi_{\alpha G}^*(x) \quad , \quad \phi^+(\beta) = \sum_{\alpha} C_\alpha^+ \Delta_{\alpha\beta} \quad , \tag{2}$$

$$\psi(x) = \sum_{KG} a_{KG} \varphi_{KG}(x) + \sum_{\alpha G} b_{\alpha G} N_\alpha \varphi_{\alpha G}(x) \quad , \quad \phi(\beta) = \sum_{\alpha} C_\alpha \Delta_{\alpha\beta} \quad ,$$

where $a_{KG}^+, a_{KG}, b_{\alpha G}^+, b_{\alpha G}$ are the Fermi operators of creation and annihilation of electrons in states $(\vec{K},G)$ and (α,G), respectively; C_α^+, C_α are the Pauli (or Fermi) operators of creaction

and annihilation of an adatom ion at adsorption centre $\vec{R}_\alpha = \alpha$; $N_\alpha = C_\alpha^+ C_\alpha = 0,1$; $\Delta_{\alpha\beta} = \Delta_{\vec{R}_\alpha, \vec{R}_\beta}$ is Kronecker symbol. Index α runs over all possible adsorption centres of surface. The symbol $\Delta_{\alpha\beta}$ is introduced for the description of configurations of adatoms over surface. The functions $\varphi_{\vec{K}G}(X)$ describe the states of electrons in metal substrate

$$\varphi_{\vec{K}G}(X) = \varphi_{\vec{K}}(\vec{x}) \Delta_{\alpha e G} \quad ; \quad \alpha e, G = \pm 1 \quad ; \quad X = \{\vec{x}, \alpha e\} \quad .$$

Here symbol $\Delta_{\alpha e G}$ describes the spin state of an electron, $\varphi_{\vec{K}}(\vec{x})$ is the wave-function of an electron moving in pure metal with quasi-momentum $\vec{K}$. In the simplest case the function $\varphi_{\vec{K}}(\vec{x})$ satisfies the following spectrum problem:

$$\left[-\frac{\hbar^2}{2m} \vec{\nabla}_x^2 - u_{cr.}(\vec{x}) \right] \varphi_{\vec{K}}(\vec{x}) = \epsilon_{\vec{K}} \varphi_{\vec{K}}(\vec{x}) \quad , \qquad (3)$$

where $u_{cr}(\vec{x})$ is the potential of the periodic crystal field of the metal substrate. It involves boundary conditions on surface. Its microscopic calculation is a complex self-consistent problem. Parameter $\epsilon_{\vec{K}}$ is the one-electron energetic spectrum of metal with a free surface; $\vec{K} = \{k_x, k_y, k_z\}$, $k_z = (0, \pi/a)$ is a lattice constant. In ref.[4] it is shown how to construct the solutions of eq. (3) by using the corresponding solutions $\varphi_{\vec{K}}(\vec{x})$ of the bulk problem. As usual, we limit ourselves to a simple electron band and neglect surface states. The additional orthonormal orbitals $\varphi_{\alpha G}(X)$ describe the electron states localized at impurities

$$\varphi_{\alpha G}(X) = \psi_\alpha(\vec{x}) \Delta_{\alpha e G} \quad ; \quad \psi_\alpha(\vec{x}) = A^{-1} \sum_\beta S_{\alpha\beta} \left[\varphi_\beta(\vec{x}) - \sum_{\vec{K}} \langle \vec{K}|\beta\rangle \varphi_{\vec{K}}(\vec{x}) \right],$$

where
$$(4)$$

$$A = \left[1 - \sum_{\vec{K}} |\langle \vec{K}|\alpha\rangle|^2 \right]^{1/2} , \quad \langle \alpha|\vec{K}\rangle = \int d\vec{x} \, \varphi_\alpha^*(\vec{x}) \, \varphi_{\vec{K}}(\vec{x}) \quad .$$

The function $\varphi_\alpha(\vec{x}) = \varphi(\vec{R}_\alpha - \vec{x})$ satisfies the following Schrödinger equation

$$\left[-\frac{\hbar^2}{2m} \vec{\nabla}_x^2 - v(\vec{x}) \right] \varphi(\vec{x}) = E \varphi(\vec{x}) \quad , \qquad (5)$$

where E is the energy of the ground state of the valence electron (or ionization potential of adatom). The functions $\psi_\alpha(\vec{x})$ are formed of the atomic orbitals $\varphi_\alpha(\vec{x})$ and $\varphi_{\vec{K}}(\vec{x})$ by taking into account the nonorthogonality pairs $\varphi_{\vec{K}}(\vec{x}), \varphi_\alpha(\vec{x})$ and $\varphi_\alpha(\vec{x}), \varphi_\beta(\vec{x})$

between themselves, i.e. $\langle \alpha|\vec{K}\rangle \neq 0$; $\langle \alpha|\beta\rangle \neq 0$. According to ref.[5], the matrix $S_{\alpha\beta}$ can be expanded over the enveloping parameters $\langle \alpha|\beta\rangle$ in the form

$$S_{\alpha\beta} = \Delta_{\alpha\beta} - \frac{1}{2} \left[1 - \Delta_{\alpha\beta} \right] \langle \beta|\alpha\rangle + \frac{3}{8} \sum_\gamma \langle \beta|\gamma\rangle \langle \gamma|\alpha\rangle (1 - \Delta_{\beta\gamma})(1 - \Delta_{\alpha\gamma}) + \cdots \quad (6)$$

The second quantization of model (1) which is constructed on the fields Ψ , Φ leads to the following expression for Hamiltonian (1)

$$H = \sum_\alpha u(\vec{R}_\alpha) N_\alpha + \frac{1}{2} \sum_{\alpha \neq \beta} N_\alpha N_\beta v(\vec{R}_\alpha - \vec{R}_\beta) - \sum_\alpha \int dX \, \Psi^+(X) \times$$
$$\times \Psi(X) N_\alpha v(\vec{R}_\alpha - \vec{x}) + \int dX \, \Psi^+(X) \left[-\frac{\hbar^2}{2m} \vec{\nabla}_x^2 - u(\vec{x}) \right] \Psi(X) + \quad (7)$$
$$+ \frac{1}{2} \int dX dX' \, \Psi^+(X) \Psi^+(X') \Psi(X') \Psi(X) v(\vec{x} - \vec{x}') \quad ,$$

where

$$\int dX = \sum_{\alpha e} \int d\vec{x} \cdots \quad .$$

Using the representation (2) of fields $\Psi(X)$, $\Phi(\beta)$, and the corresponding spectral problems (3)-(5), we may calculate the matrix elements in the Hamiltonian (6)

$$H = \sum_{\vec{K}} \epsilon_{\vec{K}} n_{\vec{K}G} + \sum_{\alpha G} N_\alpha \left\{ E_\alpha n_{\alpha G} + \frac{1}{2} U n_{\alpha G} n_{\alpha - G} \right. \quad (8)$$
$$+ \sum_{\vec{K}} \left[v_{\alpha\alpha\vec{K}} n_{\alpha - G} b_{\alpha G}^+ a_{\vec{K}G} - V_{\alpha\vec{K}} b_{\alpha G}^+ a_{\vec{K}G} + H.C. \right] \right\} +$$
$$+ \sum_{\vec{K}\vec{K}'GG'\alpha \neq \beta} N_\alpha N_\beta v_{\alpha\vec{K}\beta\vec{K}'} b_{\alpha G}^+ a_{\vec{K}G}^+ b_{\beta G'} a_{\vec{K}G} + H^{**} + C \quad .$$

Here we used the notation

$$C = -\frac{1}{2} \int d\vec{x} \, u^{(e)}(\vec{x}) \rho(\vec{x}) \quad ,$$

$$H^{**} = H_{pol.} + H_{met.} + H_{rest} \quad ,$$

$$H_{pol} = \sum_\alpha N_\alpha \left[u(\vec{R}_\alpha) - \sum_{\vec{K}\vec{K}'G} V_{\vec{K}\vec{K}'}(\alpha) a_{\vec{K}G}^+ a_{\vec{K}'G} \right] + \sum_{\alpha G} N_\alpha n_{\alpha G} \times$$

$$\times \left[\sum_{\vec{K}\vec{K}'G'} v_{\alpha\vec{K}\vec{K}'\alpha} a_{\vec{K}G}^+ a_{\vec{K}'G'} - u_{\alpha\alpha}^{(e)} - P_{\alpha\alpha} \right] + \sum_{\alpha \vec{K}G} N_\alpha \left[\sum_{\vec{K}_1 \vec{K}_2 G'} \times \right.$$

$$\times \, \mathcal{v}_{\alpha \vec{K}_1 \vec{K}_2 \vec{K}} \, a^+_{\vec{K}_1 G'} a_{\vec{K}_2 G'} - \mathcal{u}^{(e)}_{\alpha \vec{K}}) \, b^+_{\alpha G} a_{\vec{K} G} + H.C. \Big] + \frac{1}{2} \sum_{\alpha \neq \beta} N_\alpha N_\beta \Big[\mathcal{v}(\vec{R}_\alpha - \vec{R}_\beta)$$

$$- 2 \sum_{G'} n_{\alpha G'} V_{\alpha \alpha}(\beta) + \sum_{G G'} n_{\alpha G} n_{\beta G'} \, \mathcal{v}_{\alpha \beta \beta \alpha} \Big] + \sum_{\vec{K} \alpha \neq \beta G} N_\alpha N_\beta \Big[b^+_{\alpha G} \times$$

$$\times \, a_{\vec{K} G} \Big(\sum_{G'} n_{\beta G'} \mathcal{v}_{\alpha \beta \beta \vec{K}} - V_{\alpha \vec{K}}(\beta) \Big) + H.C. \Big] +$$

$$+ \sum_{\alpha \neq \beta} N_\alpha N_\beta \Big[\sum_{\vec{K}_1 \vec{K}_2 G'} \mathcal{v}_{\alpha \vec{K}_1 \vec{K}_2 \beta} \, a^+_{\vec{K}_1 G'} a_{\vec{K}_2 G'} - \mathcal{u}^{(e)}_{\alpha \beta} - P_{\alpha \beta} \Big] b^+_{\alpha G} b_{\beta G} \quad ,$$

$$H_{met} = \sum_{\alpha \neq \beta, G} N_\alpha N_\beta \Big[E_{\alpha \beta} + \mathcal{v}_{\alpha \beta \beta \beta} \, n_{\alpha - G} + \mathcal{v}_{\alpha \beta \beta \beta} \, n_{\beta - G} \Big] +$$

$$+ \frac{1}{2} \sum_{\alpha \neq \beta, G G'} N_\alpha N_\beta \, \mathcal{v}_{\alpha \beta \alpha \beta} \, b^+_{\alpha G} b^+_{\beta G'} b_{\alpha G'} b_{\beta G} \quad ,$$

$$H_{rest} = \frac{1}{2} \int dx \, dx' \, \Psi^+_{\Sigma}(x') \Big[\Psi^+_{\Sigma}(x) \Psi_{\Sigma}(x) \, \mathcal{v}(\vec{x} - \vec{x}') - 2 \mathcal{u}^{(e)}(\vec{x}) \Big] \Psi_{\Sigma}(x') -$$

$$- C + \sum_{\alpha \vec{K}_1 \vec{K}_2 G G'} N_\alpha \, \mathcal{v}_{\alpha \vec{K}_1 \alpha \vec{K}_2} \, b^+_{\alpha G} a^+_{\vec{K}_1 G'} b_{\alpha G'} a_{\vec{K}_2 G} + \sum_{\alpha \neq \beta, \vec{K} G G'} N_\alpha N_\beta \times$$

$$\times \Big[\mathcal{v}_{\alpha \alpha \beta \vec{K}} \, b^+_{\alpha G} b^+_{\alpha G'} b_{\beta G'} a_{\vec{K} G} + \mathcal{v}_{\alpha \beta \alpha \vec{K}} \, b^+_{\alpha G} b^+_{\beta G'} b_{\alpha G'} a_{\vec{K} G} $$

$$+ \frac{1}{2} \sum_{\vec{K}_1}' \mathcal{v}_{\alpha \beta \vec{K} \vec{K}_1} \, b^+_{\alpha G} b^+_{\beta G'} a_{\vec{K} G'} a_{\vec{K}_1 G} + H.C. \Big] +$$

$$+ \frac{1}{2} \sum_{\alpha \vec{K}_1 \vec{K}_2 G} \Big[\mathcal{v}_{\alpha \alpha \vec{K}_1 \vec{K}_2} \, b^+_{\alpha G} b^+_{\alpha - G} a_{\vec{K}_1 - G} a_{\vec{K}_2 G} + H.C. \Big] \quad ,$$

where

$$E_\alpha = - V_{\alpha \alpha}(\alpha) + \frac{1}{A^2} \sum_{\beta \beta'} S^*_{\alpha \beta} S_{\alpha \beta'} \, \mathcal{E}_{\beta \beta'} \quad ,$$

$$E_{\alpha \beta} = - V_{\alpha \beta}(\alpha) - V_{\alpha \beta}(\beta) + \frac{1}{A^2} \sum_{\beta' \beta''} S^*_{\alpha \beta'} S_{\beta \beta''} \, \mathcal{E}_{\beta' \beta''} \quad (\alpha \neq \beta) \quad ,$$

$$\mathcal{E}_{\beta \beta'} = \langle \beta | \beta' \rangle E - W_{\beta \beta'}(\beta') - \sum_{\vec{K}} \langle \beta | \vec{K} \rangle \, \epsilon_{\vec{K}} \, \langle \vec{K} | \beta' \rangle \quad ,$$

$$U = \int d\vec{x} \, d\vec{y} \, \mathcal{v}(\vec{x} - \vec{y}) \, \Psi^2_\alpha(\vec{x}) \, \Psi^2_\alpha(\vec{y}) \quad , \qquad P_{\beta \beta'} = \int d\vec{x} \, \varphi^*_\beta(\vec{x}) \, \varphi_{\beta'}(\vec{x}) \, \mathcal{u}_{cr}(\vec{x})$$

$$P_\beta = P_{\beta \beta} \quad , \quad W_{\beta \beta'}(\vec{R}) = \int d\vec{x} \, \varphi^*_\beta(\vec{x}) \, \varphi_{\beta'}(\vec{x}) \, \mathcal{v}(\vec{R}_\beta - \vec{x}) \quad , \quad \mathcal{u}^{(e)}(\vec{x}) = \mathcal{u}(\vec{x}) - \mathcal{u}_{cr}(\vec{x})$$

$$\Psi^+_\Sigma(x) = \sum_{\vec{K} G} \varphi^*_{\vec{K} G}(x) a^+_{\vec{K} G} \quad , \qquad \Psi_\Sigma(x) = \sum_{\vec{K} G} \varphi_{\vec{K} G}(x) a_{\vec{K} G} \quad .$$

The interaction constants $\mathcal{v}_{\alpha \vec{K} \beta \vec{K}'}$, $V_{\alpha \vec{K}}(\beta)$, $V_{\vec{K} \vec{K}'}(\alpha)$, ... etc. are the matrix elements calculated for the Coulomb interaction over the states $\Psi_\alpha(\vec{x})$, $\varphi_{\vec{K}}(\vec{x})$, ... For instance,

$$V_{\alpha \vec{K}}(\beta) = \int d\vec{x} \, \Psi^*_\alpha(\vec{x}) \, \varphi_{\vec{K}}(\vec{x}) \, \mathcal{v}(\vec{R}_\beta - \vec{x}) \quad , \qquad V_{\alpha \vec{K}} = V_{\alpha \vec{K}}(\alpha) \quad ,$$

$$V_{\vec{K} \vec{K}'}(\alpha) = \int d\vec{x} \, \varphi^*_{\vec{K}}(\vec{x}) \, \varphi_{\vec{K}'}(\vec{x}) \, \mathcal{v}(\vec{R}_\alpha - \vec{x}) \quad , \qquad \ldots \ldots \ldots \ldots \quad ,$$

$$\mathcal{v}_{\alpha \vec{K} \beta \vec{K}'} = \int d\vec{x} \, d\vec{y} \, \mathcal{v}(\vec{x} - \vec{y}) \, \Psi^*_\alpha(\vec{x}) \, \varphi^*_{\vec{K}}(\vec{y}) \, \Psi_\beta(\vec{y}) \, \varphi_{\vec{K}'}(\vec{x}) \quad , \quad \ldots \quad .$$

The function $\varphi(\vec{x})$ is the equilibrium electrom density of the pure metal substrate $\varphi(\vec{x}) = \sum_{\vec{K} G}' |\varphi_{\vec{K}}(\vec{x})|^2$ where the summing is over all the occupied states of the electron band. The latter $H.C.$ mean the Hermitian conjugate terms. The star over the function means the complex conjugate expression. The matrix elements $\mathcal{u}^{(e)}_{\vec{K} \alpha}$, $\mathcal{u}^{(e)}_{\alpha \beta}$,... , $\mathcal{u}^{(e)}_{\alpha \alpha}$, etc., are calculated for the potential $\mathcal{u}^{(e)}(\vec{x})$,

$$n_{\vec{K} G} = a^+_{\vec{K} G} a_{\vec{K} G} \quad , \qquad n_{\alpha G} = b^+_{\alpha G} b_{\alpha G} \quad .$$

Now we give a brief physical interpretation of various terms in the Hamiltonian (8).

In an explicit form Hamiltonian (8) contains the contributions playing the most important role in describing the thermodynamical and electronical properties of hydrogen-like coverages. They describe the effects of transforming the impurity electron levels E caused by the hybridization of adatom orbitals with the substrate electron wave-functions. Here, we have taken into account the enveloping of orbitals $\varphi_\alpha(\vec{x})$ and $\varphi_\beta(\vec{x})$ between themselves and with the waves $\varphi_{\vec{K}}(\vec{x})$. These processes lead to the creation of a tight chemical bond of adatoms with a metal substrate. Besides, we include here the indirect interaction between the adatoms caused by the electron exohange through the metal substrate /6/.

The term H^{**} involves the processes which are not usually considered in simple chemisorption models /6/. But sometimes they play an important role for self-consistent description of chemisorption.

The term $H_{pol.}$ describes the polarization properties of a metal substrate which are most important for self-consistent description

of ionic chemisorption, when there is a charge transfer between the substrate and adatoms /6/. They lead to the screening of the long-range Coulomb interaction between adatoms, so that the indirect interaction between them dominates. (When we have, only two single charges on the surface, this leads to the substitution of the Coulomb interaction by the dipole-dipole interaction between them by taking into account their image potentials). In the case of nonzero density of coverages this term can be taken into account as an energy of the impurity induced double electric layer and through the interaction between them and adatoms. Then, the renormalizations both of the energy of virtual level of impurity and the chemical potential of ionic components are observed. Moreover, $H_{pol.}$ contains also the interactions between the adatoms and double electric layer of the pure metal surface. The term $H_{met.}$ describes the metalization of chemisorbed coverge caused by enveloping of the adatom valence functions on the neighbouring adsorption centres. It leads to the dispersion of the virtual level and creation of the virtual impurity surface band, in the case of a periodic coverage arrangement /7/.

The term H_{rest} constains the exchange-correlation contributions and processes of electron scattering with the spin flipping and two electron hopping processes between adatoms and a substrate. These processes of higher order are usually neglected. When we neglect the term H_{rest} , it is necessary to introduce the constant C in Hamiltonian (8) for a correct evaluation of the ground state energy of metal to avoid double calculation of the electrostatic interaction between metal electrons.

When there is only single impurity localized at adsorption centre α on the metal surface $N_\alpha = 1$, $N_\beta = 0$, $\alpha \neq \beta$ and the nonorthogonality of the functions $\varphi_{\vec{k}}(\vec{x})$ and $\varphi_\alpha(\vec{x})$ and the term H^{**} are neglected, then Hamiltonian (8) transforms into the ordinary Anderson model /6/. We have only its small generalization here. The effects of the impurity level occupation on the hybridization are taken into account in this model

$$H = \sum_{\vec{k}G} \epsilon_{\vec{k}} n_{\vec{k}G} + E \sum_{G} n_{\alpha G} + U n_{\alpha G} n_{\alpha-G} +$$
$$+ \sum_{\vec{k}G}' \left\{ \left[v_{\alpha\alpha\vec{k}} \, n_{\alpha-G} \, b_{\alpha G}^+ q_{\vec{k}G} - V_{\alpha\vec{k}} \, b_{\alpha G}^+ q_{\vec{k}G} + H.c. \right] \right\} . \qquad (9)$$

In the general case the Hamiltonian (8) has the structure of the Ising model with respect to the variables N_α and N_β .

$$H = \sum_{\vec{k}G} \epsilon_{\vec{k}} n_{\vec{k}G} + \sum_\alpha \hat{\gamma}_\alpha N_\alpha + \frac{1}{2} \sum_\alpha \hat{\gamma}_{\alpha\beta} N_\alpha N_\beta , \qquad (10)$$

where $\hat{\gamma}_\alpha$, $\hat{\gamma}_{\alpha\beta}$ are the operator functions which are constructed from Fermi-amplitudes $b_{\alpha G}$, $q_{\vec{k}G}$, ... etc. They may be obtained by comparing expressions (10) and (8). They are the generalization of the ordinary Anderson model for the electron component. These Anderson-Ising generalized models of the type (8) allow us to develop the self-consistent theory of the electronical and thermodynamical properties of chemisorbed surface coverages using the Green-function mashinery /8/. Their electronical properties will be described by correlation functions of the type

$$\langle b_{\alpha G}^+ b_{\alpha G} \rangle , \quad \langle b_{\alpha G}^+ q_{\vec{k}G} \rangle , \quad \langle n_{\alpha G} \, n_{\beta G'} \rangle , \dots$$

The structure and thermodynamical behaviour of the ionic component will be described by correlation functions of the pure Ising type /9/

$$\langle N_\alpha \rangle , \quad \langle N_\alpha N_\beta \rangle , \dots$$

In conclusion, the author thanks prof. V.K. Fedyanin for his attention to this problem and useful discussions.

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Гавриленко Г.М.   Е17-87-277
Квантовостатистические модели
в теории субмонослойных покрытий

На основе последовательного микроскопического подхода, обобщающего идеи Боголюбова, развитые им в теории полярных металлов, строятся обобщенные модели типа Андерсона-Изинга для самосогласованного описания электронных и термодинамических свойств хемосорбированных водородоподобных покрытий кристаллических подложек простых металлов.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

Gavrilenko G.M.   Е17-87-277
Quantum Statistical Models in the Theory
of Submonolayer Coverages

In the framework of the consistent microscopic approach which is the generalization of Bogolubov's ideas in the theory of polar metal, the generalized Anderson - Ising models are constructed to be applied for a self-consistent description of the properties of chemisorbed hydrogen-like coverages of simple metal substrates.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.