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Application of the Morse potential to describe desorption processes from two-dimensional adsorbed layers

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Models of desorption from two-dimensional adsorbed layers in the approximation of the Morse potential are proposed. The relationship between the parameters of desorption kinetics and the potential of the adatom−substrate interaction in this approximation has been established. The conditions for the implementation of one or another desorption mechanism are formulated. The proposed models have been tested on the basis of experimental results on desorption kinetics for rare earth metal — Si(111) systems. The results obtained are important for a deeper understanding of the processes of desorption of metal atoms from the semiconductor surfaces which are subject to structural transformations.

Keywords: surface, adsorbed particle, Morse potential, desorption mechanism.

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Introduction

Desorption of atoms from a surface of metals and semiconductors is usually studied applying a kinetic approach. The approach includes analyzing results of thermodesorption spectroscopy and isothermal desorption spectroscopy and determining three quantitative parameters, namely, a desorption kinetics order (n), desorption activation energy (E_d) and a pre-exponential factor (C) [1,2]. In the simplest case, when an adsorbate concentration N is so low that lateral interaction in the adsorbed layer can be neglected (hereinafter these layers will be referred to as a two-dimensional ($2D$) gas), a desorption rate can be described by a first-order kinetic equation:

$$-\frac{dN}{dt} = C \cdot N \cdot \exp\left(-\frac{E_d}{k_B T}\right), \tag{1}$$

where T is a temperature, k_B is the Boltzmann constant. Using this equation, based on desorption curves, one can determine the magnitude E_d, which is equal to adatom binding energy and a pre-exponential factor

$$C = \frac{f_i}{f_0} \cdot \frac{k_B T}{h}, \tag{2}$$

where f_0 and f_i are partition functions of states of the atom that is in an adsorption position and an activated complex, respectively, h is the Planck constant. Depending on properties of the adsorption position and specific features of the desorption process, a ratio $\frac{f_i}{f_0}$ can be both smaller and higher than unity by several orders of magnitude.

With an increase of the surface concentration N, lateral interaction in the adsorbed layer starts playing an increasingly significant role. It results in $2D$-phase transitions on the surface, for example, a transition $2D$-gas → $2D$-islands (two-dimensional condensation) [3]. It is obvious that with this transformation desorption kinetics parameters shall be changed in the adsorbed layer as well. Indeed, it has been shown that in case of equilibrium between the islands and the $2D$-gas the desorption rate is described by a zero-order kinetic equation:

$$-\frac{dN}{dt} = C \cdot a_0^{-2} \exp\left(-\frac{E_d}{k_B T}\right), \tag{3}$$

(where a_0 is a substrate lattice constant), wherein the experimentally-obtained value of E_d is equal to energy of removal of an edge atom of the island into vacuum, while the pre-exponential factor C can in several orders exceed the similar value for the $2D$-gas (see more details below).

It is obvious from the foregoing that although the kinetics desorption parameters contain precious information about a structure of the adsorbed layer and its thermal stability, they still do not provide information about mechanisms of desorption of individual atoms. Thus, it is obvious that mechanisms of desorption from the $2D$-gas and the $2D$-islands shall have qualitative differences. At the same time, differences of the parameters E_d and C for the adsorption phases are just of a quantitative nature. Consequently, it is necessary to have an approach, which would allow specifying and analyzing atomic-level desorption processes based on the kinetic parameters.

The present study is aimed at filling the said gap at least partially and finding an interrelation between the kinetic parameters and the mechanisms of desorption. It is shown in the present study that information about these mechanisms can be obtained based on representations about the shape of a potential of interaction of the adsorbed particles with the surface, which is in turn determined by experimentally-obtained values of E_d and C for the adsorbed layer.

Presently, adsorbate−surface interaction can be described using semi-empirical Lennard−Jones and Morse potentials as well as their varieties [4]. Unlike the Lennard−Jones potential and its derivatives, which are not, strictly speaking, physically substantiated, the Morse potential was widely applied when describing various physical objects and phenomena, for example, when studying lattice dynamics, a metal defect structure, elastic properties of solid bodies, rotational-oscillatory transitions in diatomic molecules, nonlinear dynamics in biological systems, thermodynamics and transport properties of gases [5–10]. Using the Morse approximation potential, the present study has investigated a mechanism of desorption from adsorbate layers that have a various structure.

1. Results and discussion thereof

In order to solve a problem posed in the introduction, it is necessary to relate the Morse potential shape to known values of desorption kinetics for the adsorption systems, in which various structures of the adsorbed layer are realized. Besides, in order to analyze a potential type, it is necessary to have a criterion, on whose base the forms of the potential curve can be classified in the Morse approximation, thereby further enabling specifying qualitative differences of the mechanisms of the atomic-level desorption process. Therefore, first of all, we will comparatively analyze known experimental data of desorption kinetics, which have been previously obtained for rare-earth metal (REM)−silicon film structures, in which the phase transitions $2D$-gas → $2D$-islands occur.

1.1. Experimental studies of the REM−Si(111) systems: desorption kinetics parameters

Detailed data on desorption kinetics for the adsorption layers that are the $2D$-gas or the „$2D$-islands plus $2D$-gas“ system were obtained for the three systems: Yb−Si(111) [11], Eu−Si(111) [12,13] and Sm−Si(111) [14]. Formation of the adsorbed layer in the said systems is of the very similar type. Within a range of low adsorbate coverages (≤ 0.02 of a single-atom layer) and at the high temperatures of the substrates (1175−1220 K in case of Yb, 1315−1430 K in case of Eu and 1410−1490 K in case of Sm), the metal atoms form the $2D$ gas on the surface. With an increase of a coverage degree and/or slight reduction of the temperature, the phase transition $2D$-gas → $2D$-island occurs, thereby resulting in surface 3×2 reconstruction. The desorption kinetics parameters obtained for both the phases are given in Table 1.

Table 1. Desorption kinetics parameters obtained for the various phases of the adsorption systems. The data are taken from the studies [11-14]

Adsorption system	$2D$-gas		Structure (3×2) ($2D$-island)	
	E_d, eV	C^{-1}, s	E_d, eV	C^{-1}, s
Yb−Si(111)	2.9	$1 \cdot 10^{-12}$	4.4	$5 \cdot 10^{-16}$
Eu−Si(111)	3.5	$2 \cdot 10^{-12}$	4.7	$2 \cdot 10^{-15}$
Sm−Si(111)	3.2	$1 \cdot 10^{-11}$	4.95	$1.5 \cdot 10^{-16}$

When studying desorption of the REM atoms from the reconstruction (3×2), a steady-state mode was observed, i.e. the islands were in equilibrium with the $2D$-gas, thereby resulting in a zero order of desorption. It means that the experimentally-obtained value of E_d corresponds to energy of removal of the edge atom of the island into vacuum [3,15].

It is clear from analysis of the results of Table 1 that the phase transition in the adsorbed REM layer is accompanied by significant strengthening (by 1.2−1.7 eV) of a bond of the atoms with the substrate surface. This conclusion is not surprising. Indeed, according to the results obtained by means of scanning tunneling microscopy (STM) [16,17], photoelectron spectroscopy [18] and calculations based on a density functional theory (DFT) [19], formation of the $2D$-island phase is accompanied not only by origination of a long-range order in the adsorbed layer, but substantial restructuring of the silicon substrate surface as induced by the REM atoms as well. In the reconstruction 3×2, it is formed by linear honeycomb chains of Si atoms, which include unusual double π-bonds Si = Si and empty channels that lie between the silicon chains and are filled with the metal atoms (this configuration is referred in the literature to as an HCC structure). It is evident that it is non-autonomous, since it can not exist without its stabilizing adsorbate. When the REM atoms are removed from the $2D$-island, the reconstruction 3×2 is destroyed and transits into a structure that is typical for an adsorbate-uncoated surface. It all means that energy of removal of the edge atom from the island into vacuum shall be contributed not only by a summand related to disruption of bonds of the metal atom with the surface (as in the case of the single adatom), but an additional term that is to be spent for restructuring the silicon surface.

A conclusion that is at least equally important and based on data of Table 1 concerns the pre-exponential factor. As it is clear, the transition $2D$-gas → structure 3×2 is accompanied by an increase of the value of C by 3−5 orders. It is evident that such significant changes are due to the fact that desorption of the REM atoms from the $2D$-gas and the island 3×2 is most likely of a different nature. We consider this issue with more details below.

1.2. Potential energy of adsorbate–surface interaction and its interrelation with the parameters C and E_d. Criterion of selection of the model of desorption

We will assume that the values of the parameters E_d and C, on the one hand, and a kind of the Morse potential, which describes interaction of the adsorbate atom with the substrate during desorption, on the other hand, are unambiguously related to each other. It is evident that the potential shape depends on a surface condition, in particular, specific features of adsorbed particle–substrate interaction and, therefore, it can be used as a „fingerprint" for the various adsorption phases. Since a magnitude that is inverse to the parameter C has dimensionality of time (s), it is convenient to introduce the time constant $t_0 = 1/C$. As shown below, the parameter t_0 plays an important role in the Morse model and can be matched with the desorption process. The desorption kinetics data [11,13,14,20] indicate that the value of this parameter can be both higher and lower than a period of oscillations of a harmonic oscillator k_BT/h, wherein this difference can be of several orders of magnitude.

We also introduce a characteristic time t, during which the adsorbate atom transits from the unexited ground state in a potential well on the surface to a quite remote distance in vacuum (the desorption time). Then probability of desorption of the particle can be expressed as $W = t_0/t = \exp\big(-U_0/k_BT\big)$, where U_0 is potential energy of the particle in the ground unexcited state in the potential well. This equation can be rewritten as

$$t = t_0 \cdot \exp(U_0/k_BT). \tag{4}$$

It can be easily transformed into an equation for the desorption rate constant, which is obtained from a theory of absolute rates of chemical reactions: $k = 1/t = C \cdot \exp(-E_d/k_BT)$, where $E_d = U_0$.

The above consideration still does not enable constructing the models of desorption, which are other than the simplest one. It is related to present absence of a criterion that would enable differentiating physical conditions of oscillations of the desorbing atoms. The present study proposes this criterion based on comparative analysis of energy of an oscillatory quantum of the adatom $h\nu_0$, where $\nu_0 = 1/\hat{t}_0$ is an oscillation frequency, while $\hat{t}_0$ is a period of oscillations of the adatom, which can be different from the magnitude $t_0 = 1/\nu$. Based on this analysis, three qualitatively-different cases can be distinguished:

1) $\nu \approx k_BT/h$,

2) $\nu \ll k_BT/h$,

3) $\nu \gg k_BT/h$.

It is obvious that the first case corresponds to the simplest oscillation model, which can be referred to as an equilibrium one (the adatom in the potential well and the substrate lattice are in equilibrium). The relationship $t_0 \approx \hat{t}_0$ holds true. The latter means that within the framework of the kinetic model of desorption a value of $f_i/f_0 \sim 1$. The second and third cases correspond to non-equilibrium oscillation models, in which the magnitude ν for the adatom is significantly different from a frequency of thermal oscillations of the lattice. In the case 2, as shown below, the mechanism of desorption is of a resonance-step nature. It is realized, in particular, for the $2D$-gas. Finally the case 3 is opposite to the case 2 and typical for desorption from the islands. Let us consider each of the three models of desorption with more details.

1.3. Equilibrium oscillation model

Oscillations of the adsorbed particles are often represented by a simple harmonic model, in which oscillation levels are equidistant. At the same time, the spectrum data for molecule oscillations show that the oscillations are unharmonic. It should be expected that the oscillations of the adatom near the surface are also unharmonic. Therefore, it is reasonable to apply the Morse model [21] for the adsorption systems. The particle interaction potential thereof is written as

$$U(r) = D_e \cdot \big(1 - \exp\big(-a(r - r_e)\big)\big)^2, \tag{5}$$

where D_e is a depth of the potential well, r is a current distance from the surface, r_e is an equilibrium distance from the surface and a is a parameter of dimensionality of a reciprocal distance, whose value determines a width of the potential well. Various options of a graph of this curve at the same value $r_e = 5$ Å and different values of a are shown in the figure.

The model of harmonic oscillations does not provide limitations on energy of excitation of the adsorbed particle. At the same time, the Morse model has a limited number of levels in the potential well. The highest of them has energy $E_{n_m} \approx D_e$, where $n_m = \frac{2D_e - h\nu_0}{h\nu_0}$ is a level number, $\nu_0 = \frac{a}{2\pi} \cdot \sqrt{\frac{2D_e}{m}}$ is a frequency of oscillations of the adatom of the mass m. The level next to it is already a continuum level and the Morse model can not be applied within this range of energies. The typical Morse curve is shown in the figure, the curve *1*.

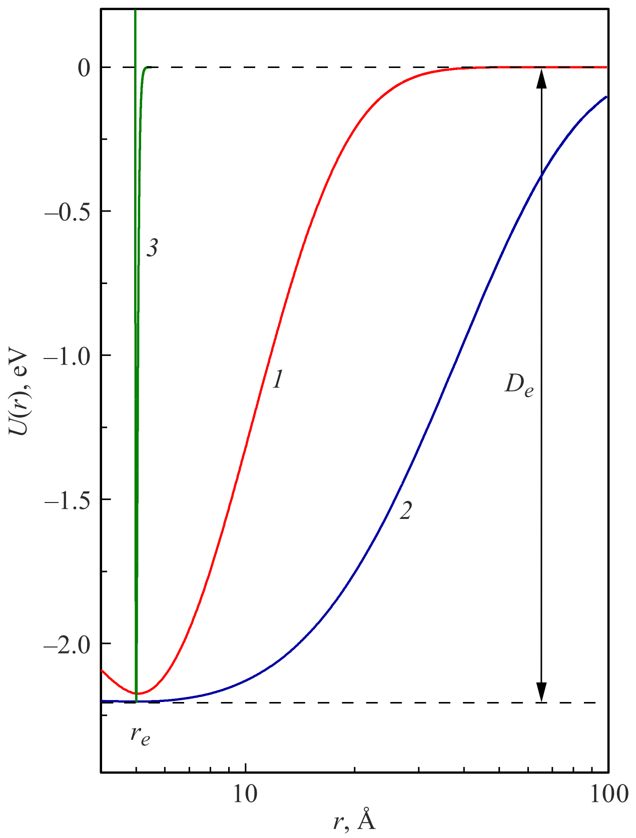
Let us consider the desorption kinetics data (the formula (4)) in the approximation of the Morse potential:

1) $U_0 = D_0 = E_d$; here the parameter D_0 characterizes a position of a zero level of oscillations as counted from the vacuum level. It is clear that $D_0 < D_e$;

2) we assume that desorption happens from the level E_{n_m}, wherein the distance of the adatom from the surface is $x_0 + r_e$, where x_0 is calculated from correspondence of t_0 to a period of oscillations of the atom of the mass m (ν_0 in the Morse model):

$$x_0 = -\frac{1}{a} \cdot \ln\left(1 - \sqrt{1 - \left(\frac{ha}{4\pi}\right)^2 \frac{1}{2D_e m}}\right). \tag{6}$$

The magnitude x_0 is a point of intersection of the Morse curve with the last oscillation level of the Morse model.



Morse curves for the various models of desorption: *1* — $a \approx 2 \cdot 10^{10}\,\mathrm{m}^{-1}$, *2* — $a \approx 2 \cdot 10^{8}\,\mathrm{m}^{-1}$, *3* — $a \approx 2 \cdot 10^{13}\,\mathrm{m}^{-1}$.

Then we obtain a simple model of desorption of the atom in one oscillation and a desorption boundary at the distance $x_0 + r_e$ as well as a parameter „a“ of the Morse model, which is approximately $\frac{1}{x_0}$.

1.4. Resonance-step model of desorption

Now, let us analyze the case when $\nu \ll k_B T/h$. It corresponds to the resonance-step model of desorption that occurs in several oscillations. Let us assume that the first oscillation occurs at the lower level of energy. When the atom returns to the surface, the adatom is excited by the oscillatory surface quantum with average energy $U = k_B T$ and transits into the next level of energy and oscillates on it till the next return to the surface. Near the surface, the atom is again excited by the quantum with energy $k_B T$ and in this way it stepwise gets to the level of energy E_{n_m}, from which it is desorbed. Implementation of this process requires that $n_m \gg \frac{E_{n_m}}{k_B T} = \ln W$. In case of implementation of such resonance-step excitation, the experimentally-observed value of t_0 is written as

$$\frac{t_0}{\hat{t}_0} = 1 + w_1 + \dots + w_n + \dots + w_{n_m} = (n_m + 1) = \frac{2D_e}{h\nu_0}, \qquad (7)$$

where w_n is probability for the particle to stay at the level n, which is numerically equal to $w_n = t_n \cdot \nu_n$, where ν_n is a frequency of oscillations of the atom at the level n and t_n is a lifetime of the particle at the level n. Since $t_n \approx h/\Delta E_{n0}$, where $\Delta E_{n0} = E_n - E_0$ is a remainder of energies of the Morse levels, then $w_n = E_n/\Delta E_{n0} = 1 + o(1)$. Whence, we obtain an estimate of the frequency

$$\hat{t}_0 = \sqrt{\frac{h t_0}{2D_e}}. \qquad (8)$$

The figure (the curve *2*) shows a typical Morse curve that corresponds to the resonance-step model of desorption, if assuming that the frequency of oscillations of the atom is ν. If the frequency of oscillations is described by the formula (8), then this case is matched with the curve *1*.

It is easy to obtain from the formula (8) an interrelation of t_0 and D_e, which explains a phenomenon that is referred in the literature to as a compensation effect of interdependence of the kinetic desorption parameters E_d and C [22].

In our experiments, the case of resonance-step desorption is matched with desorption from the $2D$-gas, whose calculation results are provided in Table 2.

1.5. Desorption from the narrow potential well

In case of implementation of the condition $\nu \gg k_B T/h$, desorption is characterized by exit of the particle from the narrow potential well with a low number of oscillation levels. The value of the parameter a is that an adsorption bond is disrupted near the state of equilibrium of the molecule near the surface, i.e. when $x_0 \ll 1\,\text{Å}$ (see the figure, the curve *3*). This situation is realized for the $2D$-islands, whose experimental data are provided in Table 1. These data and the above-given formulas were used to obtain the Morse model parameters given in Table 3. It should be noted that when calculating the depth of a desorption well by the formula (4) D_e was reduced by zero-level energy $E_0 = h/(2\hat{t}_0) - \big(h/(2\hat{t}_0)\big)^2/(4D_e)$, and $t_0 = \hat{t}_0$. The parameter x_0 was calculated by the formula

$$x_0 = -\frac{1}{a} \cdot \ln\left(1 - \sqrt{1 - \frac{D_0}{D_e}}\right), \qquad (9)$$

where $D_0 = D_e - E_0$.

The calculations have also used the parameter $C_*^{-1} = t_0$. It is in six times smaller than the parameter C^{-1} of Table 1. Using the magnitude C_* in the present study is related to the fact that the studies [11–14] have used a value of the substrate lattice constant (i.e. Si(111)(1 × 1)) as the parameter a_0 according to the models [16,17,19], whereas describing the process of desorption from the structure 3 × 2 shall take into account that an area of the lattice cell 3 × 2 is in six times higher than that of the cell (1 × 1) and that a number of adsorption locations in this structure is in six times smaller than the similar magnitude for the surface 1 × 1.

Table 2. Physical parameters of desorption for REM from the $2D$-gas

System	E_d, eV	C^{-1}, s	n_m	D_e, eV	r_e, Å	$\hat{t}_0$, s	T, K	t, s
Yb–Si(111)	2.9	$1 \cdot 10^{-12}$	37	2.98	0.38	$2.6 \cdot 10^{-14}$	1195	1.7
Eu–Si(111)	3.5	$2 \cdot 10^{-12}$	57	3.56	0.56	$3.35 \cdot 10^{-14}$	1350	23.3
Sm–Si(111)	3.2	$1 \cdot 10^{-11}$	129	3.22	1.33	$8.3 \cdot 10^{-14}$	1425	2.28

Table 3. Physical parameters of desorption for REM at the edge of the island films

System	E_d, eV	C_*^{-1}, s	n_m	D_e, eV	r_e, Å	T_1, K	t_1, s	T_2, K	t_2, s
Yb–Si(111)	4.4	$3.3 \cdot 10^{-18}$	0	349	0.00053	1150	64	1195	12
Eu–Si(111)	4.7	$8.3 \cdot 10^{-17}$	0	22.7	0.0038	1295	163	1350	29
Sm–Si(111)	4.95	$1.1 \cdot 10^{-17}$	0	117	0.0011	1340	46	1425	3.6

Note. The temperature T_1 corresponds to a flow of particles from the islands $1 \cdot 10^{12}\,\text{cm}^{-2}\text{s}^{-1}$. The temperature T_2 corresponds to the flow of particles from the islands $6 \cdot 10^{12}\,\text{cm}^{-2}\text{s}^{-1}$.

In this case the parameter $n_m = 0$ and the potential Morse well includes only the ground level. This state is long-lived, the time t is high. Besides, desorption originates restructuring of the Si(111) surface for a short period of time.

In both the tables, the Morse model's parameter r_e was estimated from the Lennard–Jones model for an attracting branch of the curve by the formula [23]:

$$y(r) = \min(r_e) \sum_r \left| \left(\left(\frac{r_e}{r}\right)^{12} - 2\left(\frac{r_e}{r}\right)^{6} \right) - \Big(\exp\big(-2a(r - r_e)\big) - 2\exp\big(-a(r - r_e)\big) \Big) \right|. \quad (10)$$

Here $r_e \le r \le x_0$, where x_0 is estimated by the formula (9). Applicability of this approach is based on the fact that the attracting branch of the Lennard–Jones potential is physically substantiated as Van der Waals forces between the surface and the atom. The values of r_e for the island films are confirmed by STM experiments [16,17] and calculations based on the density functional theory (DFT) [19], which distinctly show that the REM atoms are considerably embedded into the silicon surface (they can be even by 0.35 Å lower than the upper layer of the silicon atoms in the HCC structure). Also of note are the values of D_e in Table 3. It should be underlined that such high values of this parameter characterize not energy required for exit of the edge atom of the island into vacuum, but rather the shape of the potential Morse curve, in particular, they are related to its width. Therefore, this parameter reflects specific features of this mechanism of desorption, rather than strength of the adsorption bond of the metal atom in the structure 3×2.

1.6. Criterion of applicability of the Morse potential for describing desorption of the atoms from the surface

The last note of the present study is dedicated to an issue of applicability of the Morse potential for desorption simulation.

A specific feature of the model is a value of a reduced mass for the particle near the surface: $\mu = m \cdot M/(M + m) \approx m$, where m is a mass of the adatom and M is a total mass of all the surface atoms.

The second specific feature is presence of a flat surface, perpendicular to which desorption occurs. This enables using the one-dimensional Morse potential for analyzing the situation.

Conclusion

We have proposed and analyzed the three models for describing the desorption processes in the systems „adsorbed layer-substrate“ in the approximation of the Morse potential. It was shown on the example of the REM-Si(111) film systems that the Morse potential parameters for the adsorbed atom can be unambiguously determined from the known desorption kinetics data, i.e. n, E_d and C. The three particular cases have been considered, wherein each of them is characterized by an individual mechanism of desorption of the atom. Provided that $h\nu \approx k_B T$ the desorption process is described within the framework of the simple single-stage model of equilibrium oscillations of the particle on the surface, in which the adsorption bonds are disrupted in one oscillation and the desorption boundary is $x_0 \sim 1-10$ Å. When $h\nu \ll k_B T$, a good description for describing the desorption process is a resonance-step model, in which exit of the particle into vacuum is multi-staged and its energy increases in small batches that are equal to k_BT subsequently during transitions from underlying oscillatory levels to overlying ones in the potential well. This mechanism is typical for desorption from the $2D$-gas. At last, provided that $h\nu \gg k_BT$, the desorption nature is characterized by exit of the particle from the narrow potential well with a low number of the oscillatory levels (even with a single level) and the adsorption bond is disrupted near its equilibrium position on the surface ($x_0 \ll 1$ Å). This mechanism is typical for desorption from the $2D$-islands that are in equilibrium with the $2D$-gas on the surface.

Conflict of interest

The authors declare that they have no conflict of interest.

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