CALCULATION OF HENRY' S CONSTANTS OF ADSORPTION OF NOBLE GASES ON IDEALIZED SURFACE OF TALC

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The proportionality constants between the gas pressure and occupancy of the idealized talc surface were computed for noble gases Helium, Neon, Argon, Krypton and Xenon covering the temperature range 100 K – 450 K. Interaction potential noble gas atom – solid phase was calculated using summations of interaction potentials of Lennard-Jones type. The values of Henry's constants of adsorption were calculated using known formula based on computation of configuration integral. The one-particle configuration integral was calculated using the classical mechanics limit. The assumption of ideality of both, free gas and adsorbed phase, was used. The obtained values of Henry's constant are in qualitative agreement with the values estimated from experimental adsorption isotherms for analogical systems.

INTRODUCTION

Recently, the number of papers devoted to theoretical predictions of properties of silicate minerals grows significantly. As an example of extraordinary active area we can mention the study of electron structures and interaction potentials of zeolites (see reviews [1, 2] and citations therein). Concerning other types of silicate minerals, some recent papers can be mentioned, e. g. [3] concerns crystal-orbital Hartree-Fock (CO-HF) ab initio study of kaolinite; [4] contains CO-HF computation of mordenite (including the computations of isopotential areas of electrostatic potential inside the cavities); [5] is a semi-empirical EHT crystal-orbital study of various sheet silicates (talc, lizardite, kaolinite, pyrophillite) in various geometric configurations; [6] represents semiempirical INDO calculation of electron structure of cluster model of talc. As examples of theoretical computations of interaction potentials we mention papers [7, 8, 9]; these papers deal with interaction potentials of molecules with zeolitic systems. The values of electrostatic potential, generated by 2:1 layers of sheet silicates are computed in papers [10, 11, 12] using various levels of approximations.

The first serious attempt to perform a fully theoretical computation of the interaction of sheet silicate with adsorbate molecules is represented by papers [13, 14, 15]. In these papers, the electron structure of the smallest possible cluster model of montmorrillonite and the interaction potential of this model with water molecule were computed using semi – empirical quantum – chemical MINDO/3 method. The obtained interaction potentials were used for Monte-Carlo grand ensemble simulation of water vapor adsorption on montmorrillonite in the paper [15].

Despite of the effort of authors of the paper [15] (and many other authors in areas other than silicate minerals), the empirical interaction potentials are till yet generally used for adsorption studies. This is caused by the fact that any computation of sufficiently good-quality interaction potential has extraordinarily high requirements concerning the quality of the used quantum-chemical computational method. Well-parametrised semi-empirical methods of quantum chemistry are successful in description of chemical bonds, but they are not sufficient for computations of short-range dispersion-repulsive parts of nonbonding interaction potentials (in contrast to long-range electrostatic part of interacion potential which is often well described also by methods of this kind). The *ab initio* computations of interaction potentials require extraordinarily good-quality basis sets plus inlcusion of correlation effects. Therefore, their computing resource demands are (especially in area of silicate minerals) prohibitive also in the era of high-speed computers and advanced algorithms. All these facts lead to preference of the use of empirical potentials for computations of adsorption isotherms and other quantities connected with adsorption.

Zeolites represent the silicate systems for which the adsorption behaviour of various adsorbates is studied most freguently. This fact is caused by enormous importancy of this topic due to applications in separation and catalysis. The experience accumulated in this area is, of course, very useful for the study of adsorbtion of other silicate systems. Both, simulation methods (Molecular Dynamics – MD and Monte Carlo – MC) and methods based on calculation of configuration integral are used. From the extensive literature we will mention only some most recent publications dealing with theoretical treatment of adsorption at zeolites. Papers [16, 17] rep-

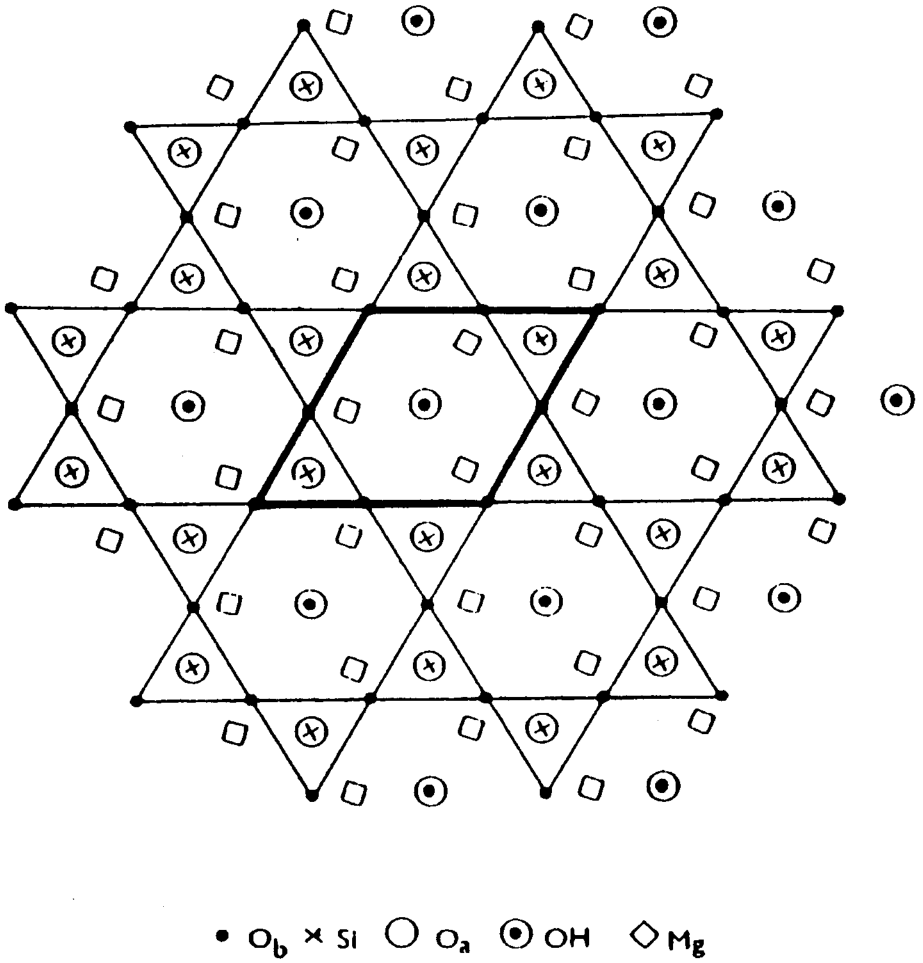


Fig. 1. The cluster model of idealized tac layer. The computation two-dimensional surface cell is drawn using thick line.

resent simulations of adsorption isotherm of noble gases in zeolite Rho using MD method. The potentials adsorbate-adsorbent and adsorbate-adsorbate are evaluated as the sum of pairwise interatomic potentials of Lennard-Jones type. The effect of electrostatic field generated by the solid is neglected. Only the contributions of surface oxygen atoms and monovalent cations are considered in the adsorbent-adsorbate potential, other atoms of the zeolite are neglected. A compensation of inaccuracies generated by these neglections is reached by such parametrisation of potential constants that the experimental value of Henry's constant is reproduced. By this way the effective potential functions were obtained. These functions are not usable for study of other systems. The parametrisation of potential constants was performed using the relation [16, 18, 21]:

$$K_1 = \frac{1}{\mathrm{k}T}\int_V \{\exp(-\Phi(\boldsymbol{r})/\mathrm{k}T) - 1\}\,\mathrm{d}\boldsymbol{r} \qquad (1)$$

where k is the Boltzmann's constant, T is the thermodynamic temperature, V is the volume considered, $\boldsymbol{r}$ is the position vector and $\Phi(\boldsymbol{r})$ is the potential energy of adsorabate in the point defined by $\boldsymbol{r}$. The potential functions for various systems are by this way obtained from experimental data, e. g. in recent papers [18, 19] are this way obtained the interaction potentials of noble gases atoms with the boron-nitride surface.

The paper [20] is an example of Monte Carlo simulation of adsorption isotherm of Xe in NaA zeolite. Grand canonical ensemble was used, potential function is a sum of interatomic Lennard-Jones potentials; the interaction of induced dipole moment in adsorbate atom with electric field generated by solid phase is explicitly included. Again, only the surface oxygens and sodium ions are taken into accound for computation of adsorbent-adsorbate potential.

MD simulation of butane and hexane in silicalite is studied in the paper [21]. The electrostatic contribution to potential is neglected. Methyle and methylene are considered as identical pseudoatoms, their interaction potential with adsorbent is computed as a sum of Lennartd-Jones potentials, silicon atoms are in this summation neglected. An important methodological aspect of the paper [21] is the volume mapping of the potential generated by adsorbent. The accuracy of the used potential parametrisation was checked by computation of Henry's constant using configuration integral evaluation method; the achieved agreement with experimental values was within 2.5%.

The computation of Henry's constant using evaluation of configurational integral is generally regarded as reference computation both for checking of potential functions and for obtaining the potential functions from experimental data as well.

The aim of the present paper is the calculation of temperature dependence of Henry's constant of adsorption of noble gases at the idealized surface of talc. Talc was the object of our interest also in our previous works [6, 12]. Thus, the calculation of Henry's constant presented in this paper characterizes in more details the quality of previous results from the point of view of interaction potentials.

METHOD

The cluster model of talc layer shown at Fig. 1 was used. This model is identical with the model used in our previous works [6, 12] for the study of electron structure of talc and study of electric potential generated by talc layer. Computational two-dimensional cell was chosen in the central part of this cluster (this cell is identical with the 2D unit cell; its translation reproduces the interaction potential generated by the infinite surface). Potential energy of noble gas atom interacting with talc layer for the area above the computational cell up to the distance 0.51 nm from the layer surface was tabulated. The tabulation was performed for the points of a rectangular grid spaced $\Delta x = 0.01$ nm, $\Delta y = 0.01$ nm, $\Delta z = 0.005$ nm. The potential was calculated as the sum of all pairwise contributions of the Lennard-Jones 6–12 type potentials between the noble gas atom in the pertinent grid point and all the atoms of the talc representing cluster. In the latter case we have used an identical cluster as the one used for the calculation of the electron structure of the talc [6]. This cluster sufficiently represents the infinite layer because the Lennard-Jones potential contains only rapidly decaying terms proportional to r^{-6} and r^{-12}:

$$\Phi^{(i)}(\boldsymbol{r}) = \sum_j \epsilon_{ij} \left[\left(\frac{\sigma_{ij}}{|\boldsymbol{r} - \boldsymbol{r}_j|} \right)^{12} - 2 \left(\frac{\sigma_{ij}}{|\boldsymbol{r} - \boldsymbol{r}_j|} \right)^{6} \right] \tag{2}$$

Table I

The used parameters of Lennard-Jones potential

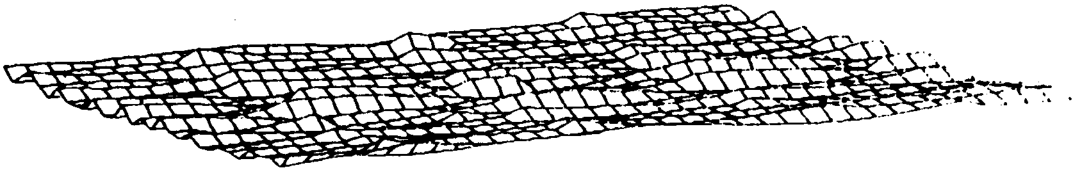
Atom pair	ϵ[kJ mol^{-1}]	σ[nm]
He – Si	0.2413	0.2855
He – O	0.1440	0.2655
He – Mg	0.2413	0.2655
He – H	0.1398	0.2655
Ne – Si	0.4499	0.2945
Ne – O	0.2689	0.3065
Ne – Mg	0.4499	0.2745
Ne – H	0.2607	0.2745
Ar – Si	0.8230	0.3305
Ar – O	0.4918	0.3425
Ar – Mg	0.4918	0.3105
Ar – H	0.4768	0.3105
Kr – Si	0.9716	0.3465
Kr – O	0.5803	0.3585
Kr – Mg	0.9716	0.3265
Kr – H	0.5630	0.3265
Xe – Si	1.1278	0.3685
Xe – O	0.6740	0.3805
Xe – Mg	1.1278	0.3485
Xe – H	0.6535	0.3485

$\Phi^{(i)}(\boldsymbol{r})$ is the potential energy of noble gas atom of type i (He, Ne, Ar, Kr, or Xe, in our case) in the point defined by position vector $\boldsymbol{r}$; j is the index of atom in the talc layer modelling cluster, $\boldsymbol{r}_j$ is the position vector of the j-th atom. Parameters ϵ_{ij} and σ_{ij} depend on the type of the noble gas atom i and the talc forming atom j. The last parameters were determined from known ϵ_{ii}, ϵ_{jj}, σ_{ii}, σ_{jj} parameters for indentical atom pairs using arithmetic and geometric combining rules, respectively. The values ϵ_{ii} and σ_{ii} commonly used for calculation of nonbonding interactions were used. Table I contains all the used parameters of Lennard-Jones potential.

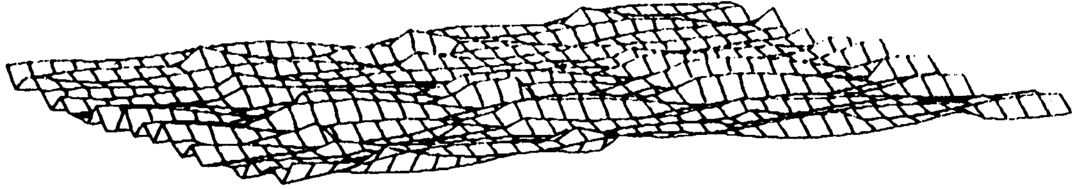
The Henry's constant is a proportionality constant between the number of adsorbed particles and the gas pressure in the limit of zero surface occupancy. In this limit the mutual interactions of adsorbed atoms can be neglected. Low occupancies of the surface are reached at low pressures; therefore, also the gas phase can be treated as an ideal one. The one-particle partition function of an atom in the ideal gaseous phase is expressed as

$$Q(\mathrm{g}) = \left(\frac{2\pi m \mathrm{k} T}{\mathrm{h}^2} \right)^{3/2} V \tag{3}$$

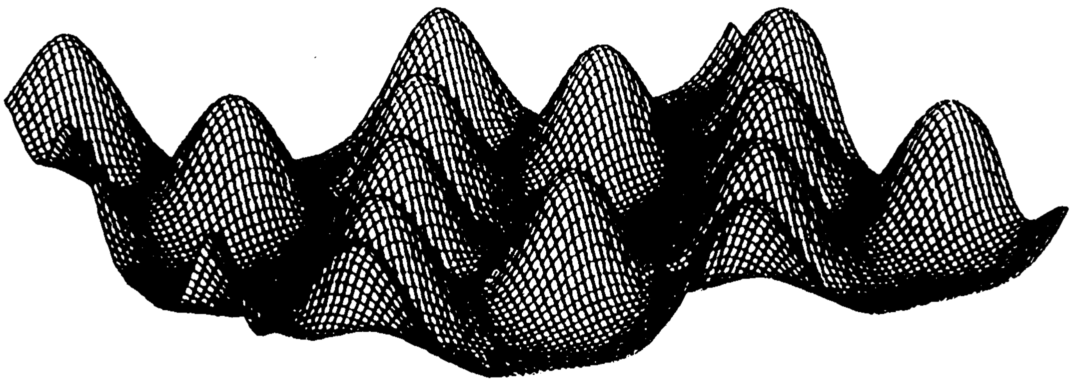
where m is the mass of the atom, k is the Boltzmann's constant, T is the thermodynamic temperature, h is



Cut 3 z = 0.400 nm



Cut 2 z = 0.350 nm



Cut 1 z = 0.285 nm

Fig. 2. The potential energy for argone atom above the talc surface. The course of the potential anergy in planes paralell with talc surface in distances 0.285 nm, 0.350 nm and 0.400 nm.

Planck's constant and V is the actual volume. The one-particle partition function for the adsorbed atom is calculated using classical mechanics limit according to relation:

$$Q(\mathrm{a}) = \left(\frac{2\pi m\mathrm{k}T}{\mathrm{h}^2}\right)^{3/2} \cdot \int_V \exp\left(-\Phi(\boldsymbol{r})/\mathrm{k}T\right) \mathrm{d}\boldsymbol{r} \qquad (4)$$

where the integration runs over the actual volume.

As mentioned above, the potential $\Phi(\boldsymbol{r})$ was tabulated in the grid points localised above the adsorbate surface. This enables the computation of configurational integral:

$$Z = \int_V \exp\left(-\Phi(\boldsymbol{r})/\mathrm{k}T\right) \mathrm{d}\boldsymbol{r} \qquad (5)$$

in the volume of tabulation. It is evident, that with the growing distance from the surface the potential $\Phi(\boldsymbol{r})$ approaches zero. The coordinate system was chosen in such a way that the adsorbent surface lies in the xy plane and the z-coordinate represents the distance from the surface. Fig. 2 shows several cuts of the potential $\Phi^{(\mathrm{Ar})}(\boldsymbol{r})$ for various values of z. Evidently, the calculated potential $\Phi(\boldsymbol{r})$ tends to flatten

Table II

The values of $z_b(i)$, $z_e(i)$, a_i and b_i

i	$z_b(i)$ [nm]	$z_e(i)$ [nm]	a_i [kJ mol^{-1}]	b_i [nm $^{-1}$]
He	0.42	0.5822	-3.68683	6.76396
Ne	0.44	0.5340	-7.17539	6.51964
Ar	0.45	0.5476	-23.82268	6.38165
Kr	0.48	0.5139	-30.24789	6.04716
Xe	0.49	0.4953	-44.25963	5.84503

Table III

Calculated values of Henry's constant of adsorption of noble gases at idelaized talc surface [pmol m^{-2}Pa^{-1}]

T [K]	He	Ne	Ar	Kr	Xe
100.0	0.227	1.321	59.823	492.910	8884.800
150.0	0.045	0.283	3.821	13.480	78.077
200.0	0.004	0.096	0.971	2.472	8.744
250.0	0.000	0.036	0.392	0.862	2.404
300.0	0.000	0.011	0.195	0.400	0.985
350.0	0.000	0.000	0.108	0.215	0.498
400.0	0.000	0.000	0.064	0.126	0.284
450.0	0.000	0.000	0.038	0.078	0.175

in the xy-plane with the increasing distance from the layer surface. Hence, for the distances greather than certain value z_b the potential can be treated as xy-independent and can be satisfactorily approximated by a function which is only z-dependent. We have used the exponential function to fit this dependence:

$$\Phi^{(i)}(\boldsymbol{r}) = \Phi^{(i)}(z) = a_i \exp(-b_i z) \quad (z \geq z_b(i)) \tag{6}$$

where by using the index i we stress that for various noble gases the constants $z_b(i)$, a_i and b_i may have different values. The actual values of a_i and b_i were determined using least-squares fit of the computed values of the tail of $\Phi^{(i)}(\boldsymbol{r})$. The values of $z_b(i)$ represent such distance from the surface at which the potential diferences throughout the considered part of xy-plane are within 1%. Using this procedure we get for the i-th noble gas the configurational integral $Z^{(i)}$ consisting of two parts:

$$Z^{(i)} = Z_{\mathrm{T}}^{(i)} + Z_{\mathrm{A}}^{(i)} \tag{7}$$

where the "tabulated part"

$$Z_{\mathrm{T}}^{(i)} = \Delta x \Delta y \Delta z \sum_{k,l,m} \exp\left(-\Phi(\boldsymbol{r}_{k,l,m})/\mathrm{k}T\right) \tag{8}$$

we obtain by numerical integration with upper limit $z_b(i)$ and the "analytic part" Z_{A} is obtained analytically:

$$Z_{\mathrm{A}}^{(i)} = \int_{z_b(i)}^{z_e(i)} \exp\left(-b_i z)/\mathrm{k}T\right) \mathrm{d}z = \tag{9}$$

$$= \frac{A}{b_i}\left\{Ei\left(-\frac{a_i}{\mathrm{k}T}\exp\left[-b_i z_b(i)\right]\right) - \right.$$

$$\left. -Ei\left(-\frac{a_i}{\mathrm{k}T}\exp\left[-b_i z_e(i)\right]\right)\right\}$$

where A is the area of the surface cell (in our case this area is 0.24303 nm^2), $z_e(i)$ represents the upper limit of the analytic integration for the noble gas of i-th type and $Ei(x)$ is the integral exponential function defined by:

$$Ei(x) = \int_{-\infty}^{x} \frac{1}{t} \exp(t) \mathrm{d}t \tag{10}$$

The total volume considered is

$$V^{(i)} = A z_e(i) \tag{11}$$

The Henry's constant was computed using the relation according to Avgul and coworkers [24]:

$$K_1 = \frac{1}{A}.\frac{Q(\mathrm{a}) - Q(\mathrm{g})}{Q(\mathrm{g})/V} \qquad (12)$$

where $Q(\mathrm{a})$ and $Q(\mathrm{g})$ are canonical one-particle partition functions of ideal gas in adsorbed (a) and gaseous (g) phase, respectively.

The values of upper limtis of analytical integration for individual noble gases $z_e(i)$ are required in (9). Such values $z_e(i)$ were chosen for which the absolute value of interaction energy (extrapolated according to (6)) is lower than 0.1% of the absolute value of the global minima of the potential $\Phi^{(i)}(\mathrm{r})$. If the upper limit of integration $z_e(i)$ is suffitiently large, the resulting value of Henry's konstant should be volume independent. This was checked by repeating the calculations using the upper limits ten-times greather than the $z_e(i)$ used.

RESULTS AND DISCUSSION

The values of $z_b(i)$, $z_e(i)$, a_i and b_i obtained using the procedure described above are in Table II. These values were used for the calculation of the analytical part of the configurational integral. Table III presents the calculated Henry's constants. The obtained values are in a qualitative agreement with the values estimated using experimental data [23]. Because of lack of suitable experimental data, we used the estimates based on data from [23]. A precise calculation of the Henry's constant based on these data is not possible; our estimates represent the possible lower limits of this quantity. The estimates for the temperature 20°C are: for Kr adsorbed at kaolinite: 2.8×10^{-14} mol $\mathrm{m}^{-2}\mathrm{Pa}^{-1}$; N_2 at talc: 9.0×10^{-14} mol $\mathrm{m}^{-2}\mathrm{Pa}^{-1}$; at kaolinite: $8{,}7 \times 10^{-14}$ mol $\mathrm{m}^{-2}\mathrm{Pa}^{-1}$. Comparison of the estimated lower limit of Henry's constant for N_2 at the talc with the computed one for Ar (1.95×10^{-13} mol $\mathrm{m}^{-2}\mathrm{Pa}^{-1}$ at 300 K) shows a qualitative agreement. Extrapolating the Henry's constant for Kr at talc from the known values for Kr and N_2 at kaolinite and N_2 at talc we get an estimate 1.2×10^{-13} mol m^{-2} Pa^{-1}. The comparison of this estimate with the calculated value 4×10^{-13} mol $\mathrm{m}^{-2}\mathrm{Pa}^{-1}$ can be interpreted – taking into account the very approximative estimate of the "experimental value" – as a qualitative agreement. The theoretical data in Table III show expected trends accordig to temperature and also according to atomic numbers.

A direct comparison of calculated and experimental data would not be possible even in the case if the experimental data were available. The theoretical data are calculated for the chemically saturated surface of the talc layer. However, real talc contains about 20% of the "broken surface" which represent the edges of the broken particles. This surface is not chemically saturated and its properties are completely different than the properties of the studied ideal surface. Its adsorption ability should be much more greather than the affinity of the smooth saturated ideal surface. Therefore, the present study is rather a theoretical model study than a direct prediction of experimentally measured values. The experimental values of Henry's constand should depend on the shape and particle size distribution function. The calculated values refer rather to surface of an ideal crystal.

CONCLUSIONS

The obtained theoretical values of Henry's constant of adsorption of noble gases at idealized talc surface show expected trends. The theoretical values are in qualitative agreement with the values estimated from experimetnal data for analogical systems. This fact indicates the suitability of the used potential functions and the suitability of the used geometric model of the talc layer. In the future, the influence of the inclusion of electric field generated by solid to the value of Henry's constant is to be examined. This question becomes extraordinarily interesting in the case of surfaces which are not electroneutral.

Acknowledgement

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VÝPOČET HENRYHO KONŠTANTY ADSORPCIE VZÁCNYCH PLYNOV NA IDEALIZOVANOM POVRCHU MASTENCA

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Vypočítali sa Henryho koštanty adsorpcie vzácnych plynov na idealizovanom povrchu jednej vrstvy mastenca v teplotnom rozsahu 100 K – 400 K. Pre výpočet sa použil štatistickotermodynamický vzťah, založený na znalosti kanonických partičných funkcií adsorbovaného i voľného plynu. Tieto partičné funkcie sa pre jednotlivé vzácne plyny interagujúce s povrchom mastenca vypočítali v klasickej limite, bez kvantových korekcií. Ako pre voľný plyn, tak aj pre adsorbované atómy sa použila aproximácia ideálneho plynu, ktorá je vzhľadom na definíciu Henryho konštanty adsorpcie (konštanta úmernosti medzi tlakom plynu a obsadením povrchu v limite pre nulové obsadenie povrchu) pre tento prípad prijateľná. Potenciálna energia interakcie atómu vzácneho plynu s izolovanou vrstvou mastenca se vyjadrila cez Lennardove-Jonesove párové potenciály. Pre výpočet sa použil 298 atómový klaster, ktorý dostatočne dobre modeluje izolovanú vrstvu mastenca. Získané hodnoty Henryho konštánt adsorpcie sú v kvalitatívnom súhlase s údajmi, odhadnutými na základe experimentálne stanovených adsorpčných izoterm pre analogické systémy.

Obr. 1. Klastrový model idealizovanej vrstvy mastenca. Hrubými čiarami je vyznačená povrchová dojrozmerná výpočtová bunka.

Obr. 2. Potenciálna energia atómu argónu nad povrchom mastenca. Priebeh potenciálnej energie v rovinách rovnobežných s povrchom mastenca vo vzdialenostiach 0.285 nm, 0.350 nm a 0.400 nm.

Book Reviews

INDEX TO SCIENTIFIC REVIEWS, 1992 First Semiannual, Institute for Scientific Information, Philadelphia, Pennsylvania 1992, ISSN 0360-0661, 2110 pages

This is and index to the review literature in all areas fo science and technology. It provides cover-to-cover indexing of 209 current review serials, as well as selective coverage of review-type articles from 2341 international journals.

Review articles proved to be of high value for scientists and scholars anabling them to maintain current awareness of present activity in their own and related fields of interest. They are useful to students in undestanding new subjects, and to specialists and researchers in continuing education or in obtaining an overwiew of a subject outside their field of specialization before commencing a new project. And, last but not least, reviews are almost invariably accompanied by comprehensive bibliographies of the primary documents reviewed, and are therefore useful as bibliographic tools in making retrospective literature searches. But the very low frequency of review articles compared to the total literature (estimated at between 3% and 4%) makes their search rather difficult and inefficient. That is why Institute for Scientific Information (3501 Market Street, Philadelphia, Pennsylvania 19104) started to produce Index to scientific Reviews (ISR) which is, in fact, the only multidisciplinary index specifically designed o help to locate review articles.

The first issue of ISR appeared in 1975, covering the review literature of 1974. Since then it appears annually in two hardbound semiannuals. Each issue includes: the Source Index, which provides complete bibliographic information for each review article (22,993 review articles are covered by the 1992 First Semiannual), and is arranged alphabetically by author, the Permuterm Subject Index, which given access to reviews by key words appearing in their titles, the Corporate Index which provides access to publishing authors and their works by corporate or academic affiliation listed in two sections – Geographic and Organization and the Research Front Specialty Index, which provides a list of all research front specialties cited by source items in the current issue of ISR (6,599 Research Front Specialty names are referred to in the 1992 First Semiannual, the average number of source items per