# Open Access Article SEPARATION BOUNDARY, BINDING ENERGY AND KINETICS OF SURFACE PROCESSES ON A SOLID

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**Abstract.** The article presents the main prefix about the structure of the crystal, the energy of interaction, the laws of surface phenomena. Energy exchange between gas atoms and the surface. The physical aspects of energy interaction are considered.

**Keywords:** crystal, surface energy, average energy, interface, lattice, valence bonds, evaporation, probability

The crystal has an equilibrium configuration, its surface will consist of the ideal planes described above only at absolute zero temperature. At finite temperatures, some of the atoms leave their equilibrium positions, and the structure of the surface becomes more complex.[1]

There is another reason for the complexity of the surface structure. The main characteristic of a solid is the immutability of its shape. This property is provided, in particular, by the very low rate of any relaxation processes in a solid associated with the movement of its constituent atoms. Therefore, in the vast majority of cases, a solid body does not have an equilibrium, but a metastable form, that is, a form that, although not stable, persists throughout the entire observation time due to the very low speed of those processes that could bring the body into an equilibrium state. In particular, the shape of the surface of a solid is determined in most cases by its prehistory (growth, processing) and can be very far from equilibrium.[2]

The simplest microscopic model that allows you to describe the structure of the real surface of a solid body is called a Kossel crystal. In this model, the crystallographic cell is replaced by a simple cubic building block. The part of the plane completely filled with such blocks is called a terrace. The

Received: October 04, 2023 / Revised: October 30, 2023 / Accepted: November 18, 2023 / Published: December 18, 2023 About the authors: Bozorov Nosirjon Sodikovich Corresponding author-Email: terraces, spread out on different levels, are connected by steps with a height of one or more cubic blocks. The steps themselves may also not be straight, but contain fractures. [3]

A block of a simple cubic shape, located inside a volume filled with the same blocks, has six nearest neighbors, with which it is in contact with faces. The block that is part of the terrace is in contact with only the five nearest neighbors, so its contribution to the interaction energy is less than that of the block that is in the volume. The block that is part of the stage has only four neighbors, and at the break of the stage – three.[4] An atom adjacent to the stage, but not part of it, has only two neighbors, and an atom lying on the terrace is in direct contact with only one block that is part of the terrace. Its interaction energy with the rest of the crystal is the lowest, and it is he who can most easily break away from the crystal and evaporate. If a solid body borders on its own equilibrium vapor, then evaporation and condensation processes constantly occur at the boundary, compensating for each other. If the vapor pressure is greater than the equilibrium one, then the crystal grows, and if it is less, it evaporates.

If a solid body borders not with its own steam, but with another gaseous medium, then the particles of this medium, which in the future we will call atoms, although they may also be molecules, will hit the surface of the solid. It is known that at long distances between an atom and a surface, attractive forces act, which are replaced by repulsion at distances comparable to the size of atoms. Thus, any atom can be held near the surface at a certain equilibrium distance corresponding to the minimum potential energy of the resultant forces of attraction and repulsion. An atom trapped in such a potential pit is called adsorbed, and its potential energy at the bottom of the pit is called the adsorption energy. Depending on the value of the adsorption energy, the physical form of adsorption and the chemical form or chemisorption are distinguished.[5]

In the physical form of adsorption, the interaction energy of the adsorbed atom with the surface is small compared to the binding energy of the atoms of the solid on which the adsorption occurred. In this case, the adsorbed atom only slightly distorts the surface structure and is easily and without consequences removed, or, as they say, desorbed, from it when heated.[6] In contrast, during chemisorption, the interaction between the atom and the surface is so strong that it turns out to be comparable to the interaction between the atoms that make up the surface of a solid. As a rule, it turns out to be impossible to destroy this connection without significantly changing the surface. [7]

Despite the fact that all atoms are attracted to the surface, the probability that adsorption will occur when an atom hits the surface is not equal to one. Another, much more likely outcome in some situations, is that the atom will hit the surface and then fly back into the gaseous medium. [8] The reason why the atom is not adsorbed, despite its attraction to the surface, is that in order to transition to the adsorbed state, the incoming atom must transfer its excess energy to the surface. The probability that adsorption will occur is called the probability of adhesion. [9]

The exchange of energy between gas atoms and a surface having different temperatures plays an important role in technology, including space technology. [10] To characterize this process, an energy accommodation coefficient is introduced, which is determined by the following formula:

$$\alpha_{\varepsilon} = \frac{E_i - E_r}{E_i - E_s} \tag{1}$$

where  $E_i$  - the average energy of atoms hitting the surface,  $E_r$  - the average energy of the atoms bounced off the surface,  $E_s$  - the average energy of the bounced atoms that they would have if the gas were in equilibrium with the surface. If the probability of sticking is high, then the coefficient of energy accommodation is approaching one. [11]

The idea of bodies with no boundaries has proved extremely fruitful in the study of the volumetric properties of condensed matter. The theory of a solid body, built for a model in which a body is considered infinitely extended or cyclic boundary conditions are artificially placed on its boundaries, turning it into an endless repetition of the same fragment, acquires completeness and simplicity. The price for these simplifications is the complexity, and sometimes the impossibility, of describing those phenomena in which the interfaces of bodies of different natures are essential. At the same time, all real bodies are limited, and surface phenomena play a crucial role in both natural and technological processes. The modern development of technology towards the miniaturization of all devices and the increasing role of nanotechnology makes understanding surface processes especially relevant. [12]

The first step towards describing spatially limited bodies is the idea of an infinitely long flat interface between two phases: a solid and a vacuum. Of course, such a state is not in equilibrium from a thermodynamic point of view, since evaporation must occur. However, provided that the equilibrium vapor pressure is low, this process is slow and we will not deal with it yet. Then, for a crystalline solid, two phenomena related to the presence of a surface come to the fore: relaxation of the surface and its reconstruction. [13]

Surface relaxation is understood as the difference between the distances between the last crystallographic planes parallel to the plane of the boundary with the vacuum from the distances between the same planes in the volume. It is assumed that the arrangement of atoms in the latter plane completely coincides with the arrangement of atoms in all other planes parallel to it. Otherwise, if the atoms of the last plane are displaced from the positions they occupy in other planes located in the volume of the material, then it is said that a surface reconstruction has occurred.

One of the common reasons for surface reconstruction is the appearance of "broken ties" on it. Thus, silicon forms crystals in which all atoms are connected to their four nearest neighbors by valence bonds. The silicon atoms on the surface are devoid of neighbors that should be in the overlying layers. The valence bonds that turn out to be free lead to a stronger interaction between atoms located in adjacent rows of the surface plane.[14] As a result, surface atoms are divided into pairs, and the distance between atoms in a pair is less than the distance between atoms belonging to neighboring pairs. Thus, surface reconstruction can lead not only to a significant displacement of surface atoms, but also to an increase (in this case, to a doubling) of the repetition period of similar elements compared with the period of the bulk lattice.[15] In some cases, there is also a change in the symmetry of the arrangement of atoms compared to what took place in the volume.

Stable condensed bodies do not spontaneously fall apart. From a physical point of view, the reason for stability is the need to perform work to form new interfaces with vacuum when dividing a body into parts. Thus, the energy of a body having a longer boundary with a vacuum exerts more than

that of a body having a less extended boundary. This additional energy is attributed to the surface area of the body and is called surface energy.

In equilibrium, the body must take a shape in which the surface energy is minimal. For liquids, this requirement is reduced to a minimum surface area for a given body volume. As it is known from mathematics, a ball has the smallest surface for a given volume, therefore, any finite volume of liquid in a free state must take the shape of a ball.

Solid crystalline bodies have a more complex equilibrium shape, since the surface energies of different crystallographic faces are not the same. In this case, the minimum surface energy is achieved not with a minimum total surface area, but with a shape that provides a large proportion for those crystallographic faces that have less surface energy.[16] If the dependence of the surface energy on the direction in the crystal is known, then the equilibrium shape of the crystal can be obtained using the Wolfe construction. From an arbitrary point taken as the center of the crystal, segments proportional to the surface energy of those planes that are perpendicular to this direction are deposited in all directions. Then the inner envelope surface of all such planes is constructed, drawn through the ends of the corresponding segments. If one of the crystal faces has a much lower surface energy than the other faces, then almost the entire surface of the crystal (with the exception of small curves near the edges) will be formed by such faces. A good example is cubic crystals of table salt, in which all six faces are formed by planes having the same structure and having the lowest surface energy. The shape of real crystals does not always coincide with the body obtained by the method described above, since crystal growth often occurs in conditions very far from equilibrium.

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