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BOUNDARY SEPARATION AND BINDING ENERGY OF ATOMS IN THE REAL SURFACE OF A SOLID

Bozorov Nasirjon Sodikovich
Kakand state pedagogical institute

Umurkulov Kayumjon Parpievich
Kakand state pedagogical institute

Alisherov Otabek Alisher son
Kakand state pedagogical institute

Abdumanonova Firuza Abdualiyevna
Tajik State University of Law

ANATATSION

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.
There is another reason for complicating the structure of the surface. The main characteristic of a solid is the immutability of its shape. This property is provided, in particular, by a very low rate of any relaxation processes in a solid body associated with the movement of its constituent atoms. Therefore, in the vast majority of cases, a solid body has not 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 transfer the body to 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.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-shaped building block. The part of the plane completely filled with such blocks is called a terrace. 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.
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 the faces of only five nearest neighbors, so that 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. The atom adjacent to the step,

but not part of it, has only two neighbors, and the 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 smallest, 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, then the crystal grows, and if less, it evaporates.

If a solid body borders not with its own vapor, but with another gas 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 the atom and the 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.

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. 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 is impossible to destroy this connection without a significant change in the surface.

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, in some situations much more likely, outcome is that the atom will hit the surface and then fly back into the gaseous medium. The reason why the atom is not adsorbed, despite the 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.

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

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

where E_i - the average energy of the atoms hitting the surface, Er is the average energy of the atoms bouncing off the surface, Es is the average energy of the bounced atoms that they would have if the gas was in equilibrium with the surface. If the probability of sticking is high, then the energy accommodation coefficient approaches unity.

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