Statistical model of atoms diffusion in a crystal lattice of a metal

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To describe the diffusion of atoms in the crystal lattice of a metal, we use the statistical model, which was previously well tested for the description of thermionic emission [1]. Atoms in the crystal lattice of a metal are held by large attractive forces, therefore the potential energy of moving, i.e. diffusing atoms is greater than the potential energy of the atoms of the crystal lattice by the value of u — the activation energy of the diffusion process.

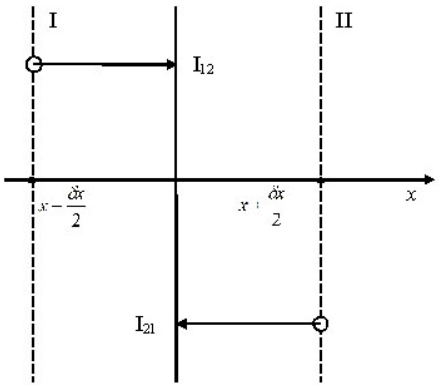

Fig. 1. Scheme of diffusion in the statistical atomic model.

Let us single out in a unit volume of metal V a unit surface perpendicular to the x axis (Fig. 1). The total flow of atoms in the positive direction of the x axis is equal to the difference in the flow I_{12} (from the plane $x - d/2$ to the plane $x + d/2$) and I_{21} (in the opposite direction) [1]. Only those metal atoms for which the energy ε is larger than the potential barrier of the lattice u can pass through this surface in the positive direction of the x axis:

$$\varepsilon = \frac{\mathrm{p_x^2}}{2\mathrm{m}} \geq u \qquad (1)$$

and m is the mass of the diffusing atom. The diffusion flow I_{12} is determined by the number of metal atoms or impurities passing through a unit of surface per unit of time. To find its expression, it is necessary to calculate the distribution of atoms by impulses:

$$dN = \frac{\mathrm{V}dp_x dp_y dp_z}{\mathrm{h}^3 \exp((\varepsilon - \mu)/kT)}. \qquad (2)$$

There, dN is the number of atoms in the metal whose pulse components are in the range of values between p_x and $p_x + dp_x$, $\mathrm{p_y}$ and $p_y + dp_y$, $\mathrm{p_z}$ and $p_z + dp_z$, i.e. number of particles with impulse and energy given in magnitude and direction, T – temperature. The number of atoms passing through a unit of surface per unit of time:

$$dn = \frac{dp_x dp_y dp_z}{\mathrm{mh}^3 \exp((\varepsilon - \mu)/kT)}, \qquad (3)$$

Performing the well-known calculations [1], we find the diffusion flow I_{12} in the direction of the x axis:

$$I_{12} = \frac{2\pi mk^2T^2}{h^3} \exp\text{-}((\mathrm{u} - \mu_1)/\mathrm{kT}) \ , \qquad (4)$$

where μ_1 is the chemical potential of metal atoms on the side of plane I (Fig. 1). Similarly, we find the diffusion flow I_{21} in the direction opposite to the x axis (from plane II to plane I). The total diffusion flow is equal to:

$$Ic = I_{12} - I_{21} = \frac{2\pi mk^2T^2}{h^3} \mathrm{e}^{-\mathrm{w/kT}} \exp((\mu_1 - \mu_2)/\mathrm{kT}) \ . \qquad (5)$$

Perform a further transformation of equation (5). If we consider the self-diffusion of atoms of a pure metal, then the difference of their chemical potential at the interplanar distance $\Delta\mu=\mu_1-\mu_2 \ll 1$, then $exp(\mu_1-\mu_2)/kT \approx (\mu_1-\mu_2)/kT$. According to the average theorem, we find the equation:

$$Ic = -\frac{2\pi mkTd}{h^3} \mathrm{e}^{-\mathrm{w/kT}} \frac{\partial \mu}{\partial x} \qquad (6)$$

It is the statistical equation of atoms diffusion in a crystal lattice of a metal. That allows us to calculate *ab initio* the zero diffusion coefficient of atoms.

References

[1] V. A. Kozheurov: Statisticheskaya termodinamika. M.: Metallurgiya, 175 (1975).