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ИЗДАНИЕ
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The Influence of Forms and Sizes of Microheterogeneous Systems on the Band Bending in AgBr-AgI

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Abstract – Nonideal heterojunction of AgBr-AgI has been considered. The Poisson equations for heterojunction in planar, spherical and cylindrical geometries have been solved in linear approximation. The expressions for band bending of heterojunctions are derived. Calculations of band bending vs. the size, forms of the core and the surface charge on the interface have been carried out.

To increase of the efficiency of transforming the photon energy into the latent image centers it is necessary to segregate electrons and holes, that is, to reduce their recombination velocity. To solve this problem methods of synthesis of silver halide microcrystals (MC) of a heterojunction type, a "core-shell", on the basis of AgBr-AgI are developed [1–3]. Silver particles in these systems upon exposure are formed on the interface. Silver halides are known to be large band-gap, disordered according to Frenkel, ionic semiconductors. In the heterojunction area of AgBr the band bending is directed downwards and in the heterojunction area of AgI – the band bending is directed upwards [4]. The thickness of the shell of AgI is 0,12 μm . The size of the core of AgBr is 0,25 – 0,4 μm and comparable with the Debye length of defects. The size of the band bending on the heterojunction interface depends both on the core size and on the form of the heterostructure. Hence, changing the form and the sizes of the "core-shell" heterosystem it is possible to govern their photosensitivity.

Let us solve the problem of the influence of the form and the size of the "core-shell" heterosystem on the band bending on the heterojunction by means of [5]. The qualitative scheme of the distribution of the potential in the heterojunction of AgBr-AgI is represented in Fig. 1, where ψ_c is the junction potential difference caused by different work functions of electrons from AgBr and AgI; $\delta\psi_1$ – the band bending in AgBr on the AgI interface; $\delta\psi_2$ – the band bending in AgI on the AgBr interface; ψ_1 – the distribution of the potential in AgBr; ψ_2 – the distribution of the potential in AgI; ψ_0 – the potential arising in the center of AgBr MC, because the volume charge in the center of the MC comparable with the Debye length is not equal to zero; h_1 – a characteristic size of the AgBr microcrystal. The ψ_c , $\delta\psi_1$, $\delta\psi_2$, ψ_1 , ψ_2 potentials and the ψ_0 are normalized on $k_B T/q$, where k_B is the Boltzmann constant, q – an elementary charge.

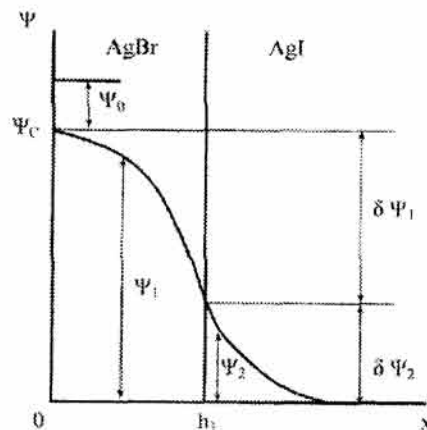


Fig. 1. Qualitative distribution of potential in AgBr-AgI heterojunction

Let us write the Poisson equations for the AgBr and AgI MC. The concentrations of electrons and holes in these compounds are small in comparison with the concentration of the Frenkel defects – interstitial silver cations and cation vacancies. The Frenkel defects in the electric field are distributed according to Boltzmann. Let us write the Poisson equations for the core and the shell in dimensionless variables

$$\Delta(\psi_c + \psi_0 - \psi_1) = \text{sh}(\psi_c + \psi_0 - \psi_1), \quad (1)$$

$$\Delta(\psi_2) = \text{sh}(\psi_2), \quad (2)$$

where

$$\Delta = \frac{1}{\xi_i^m} \frac{d}{d\xi_i} \left(\xi_i^m \frac{d}{d\xi_i} \right) \quad i = 1, 2,$$

is the Laplacian. The $i=1$ index is for the core and the $i=2$ index is for the shell. Here $\xi_i = x/l_i$ is the coordinate whose beginning is in the center of the "core-shell" system and normalized to the Debye length l_i :

$$l_i = \left(\frac{k_B \epsilon_i \epsilon_0}{2q^2 n_i} \right)^{1/2}, \quad (3)$$

where ϵ_0 is the electric constant; n_i – the equilibrium concentration of defects in a infinitely large crystal. The parameters are equal to $m=0, 1, 2$ for planar, cylindrical and spherical systems, respectively. The equations (1–2) have the following boundary conditions: – in the center of the "core-shell" system by virtue of the symmetry of the equation

$$\xi_1 = 0, \quad \frac{d\psi_1}{d\xi_1} = 0. \quad (4)$$

– besides, according to Fig. 1

At $r_1 \gg l_1, l_2$ expressions (39) and (40) for the band bendings assume the form of (24) for a flat disc. According to (39) and (40) relative changes of the band bendings are calculated with account of the core size and the charge σ . The results of the calculations are resulted in Fig. 4.

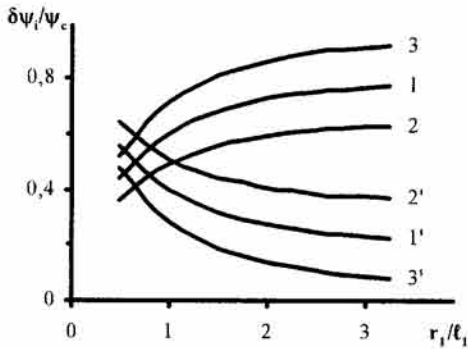


Fig. 4. Influence of the radius of the "core" in the spherical form on a band bending on the boundary of the AgBr-AgI heterojunction: $\delta\psi_1/\psi_c$ - curves 1 - 3; $\delta\psi_2/\psi_c$ - curves 1' - 3' (curves 1, 1' - $\sigma/\psi_c=0$; curves 2, 2' - $\sigma/\psi_c=-1,6 \cdot 10^{-9}$ C/cm²; curves 3, 3' - $\sigma/\psi_c=1,6 \cdot 10^{-9}$ C/cm²)

From Fig. 2-4 it is seen that increase in a characteristic size of the core results in band bendings' increase in AgBr and band bendings' decrease in AgI. At $h_1, r_1 > 3l_1$ the band bendings on the boundary of two silver halides practically do not change with increasing of a characteristic size of a core. The negative charge on the interface of the phases reduces the value of band bendings in AgBr and increases the one in AgI. The positive charge on the interface of the phases, alternatively, increases the value of band bendings in AgBr

and reduces the one in AgI. The given effect is related to electroneutrality of the "core - shell" system.

Increase in band bendings in AgBr results in increase in the negative volume charge caused by cation vacancies. Increase in band bendings in AgI results in increase in the positive volume charge caused by interstitial silver cations. Alternatively, the band bendings on the AgBr-AgI heterojunction depends not only on the size of a core, but also on the geometry of the photosensitive "core - shell" system. It is necessary to note that the band bendings for planar and spherical heterojunctions are similar, and, hence, the photosensivities of these systems must be comparable. Therefore, changing the form and the sizes of the core, it is possible to change the band bending, and, hence, to govern the photosensitivity of materials on the basis of silver halide microcrystals of a heterojunction type.

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