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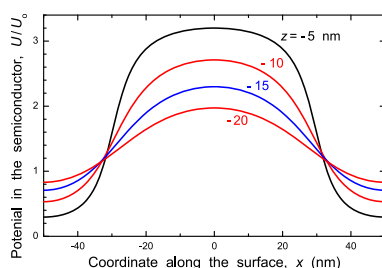
## Potential profiles near the nano-patterned semiconductor–electrolyte interface

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### HIGHLIGHTS

- The interface is considered to contain charged spots.
- The lateral size of spots is appreciably larger than the double-layer thickness.
- The potential profiles in the semiconductor are calculated for this case.
- The results are of interest in the context of electron–hole pair separation.

### GRAPHICAL ABSTRACT



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### ABSTRACT

Nanostructured semiconductor–electrolyte interfaces are of high current interest due to novel physics and potential applications. The understanding of the corresponding potential profiles is, however, lacking. Our calculations illustrate the specifics of the potential profiles in a semiconductor near the charged nano-patterned interface separating a semiconductor and electrolyte. The lateral size of patterns is considered to be appreciably larger than the double-layer thickness. Despite this condition, the potential profiles are found to change in both directions on the length scale comparable to the size of patterns. The identified gradients in the potential profiles may be useful in applications including, e.g., electron–hole pair excitation and separation.

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The understanding and quantification of what happens on the semiconductor–electrolyte interface are of considerable intrinsic interest and also technologically important. In various related applications, semiconductors are often either doped or contain relatively high concentration of defects which play a role of donors or acceptors of electrons. The conventional analysis [1] of the charge distribution in such cases implies that the interface is uniform (at least on the lateral scale larger than 1 nm) and usually

includes two well-known counterparts. The first one is the 1D Schottky model describing the charge depletion near the interface (this model was originally proposed for the semiconductor–metal junctions as reviewed in detail by Ludeke [2]). The second one is one of the models describing the double layer located on the electrolyte side (reviewed in detail, e.g., by Schmickler [3]). To link these models, the depletion length is defined by the requirement that the Fermi energy in the bulk of the semiconductor is equal to the redox potential in the electrolyte.

During the past decade, the corresponding experimental studies have often become focused on various processes occurring on semiconductor–electrolyte interfaces heterogeneous on the length scale from about 10 to 100 nm. Theoretical studies illustrating the

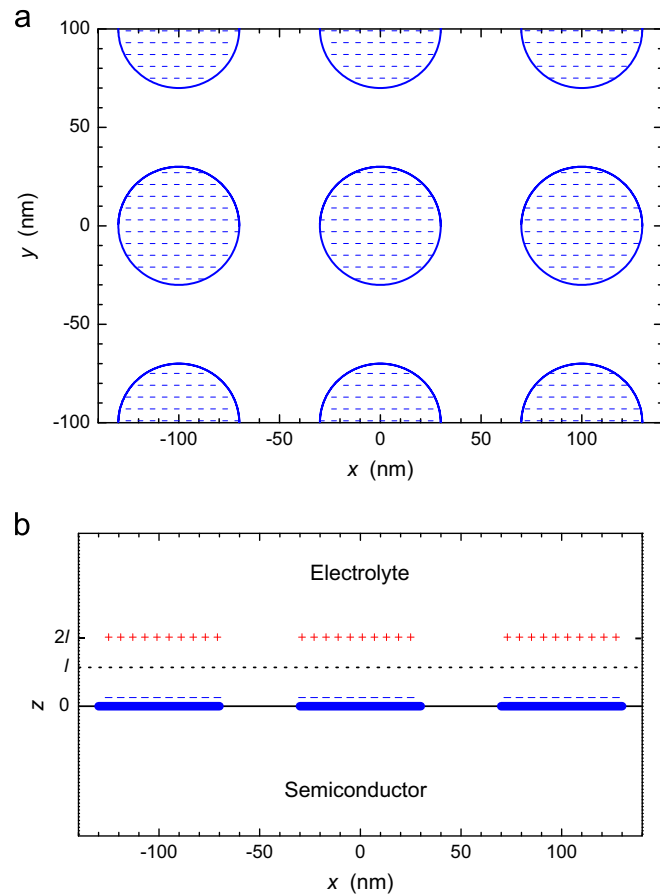
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specifics of the distribution of electric field in such cases are lacking. In analogy with the conventional 1D Schottky model, one can refer here to the models describing the mean-field potential profile near metal nanoparticles surrounded by a semiconductor or located at the semiconductor–vacuum interface (see, e.g., Refs. [4–7] and a recent detailed review by Zhang and Yates [8]). These models are, however, not directly applicable to the semiconductor–electrolyte interface, because in the latter case the charge located at the interface is screened by the electrolyte.

In this communication, we describe a simple model allowing one to understand the type of the potential profiles in a semiconductor near a heterogeneous semiconductor–electrolyte interface in one of the generic cases when a uniform semiconductor surface is periodically patterned on the 10–100 nm scale by deposition of another material. The material may be a semiconductor with high density of surface states occupied by electrons or a metal with surface charge related to the double-layer formation. The field generated by these electrons or the surface charge is screened by electrolyte. Near the interface on the semiconductor side, the screening is, however, not complete, and accordingly the potential changes in the direction perpendicular to the interface and also periodically in the directions along the interface. For example, we consider that the spots of the deposited material are circularly shaped (with radius  $R$ ) and form a square lattice (with lattice spacing  $L$ ) as shown in Fig. 1(a).

Experimentally, the structures under consideration can be fabricated by using, e.g., electron beam lithography. In particular, the deposited material can be shaped as cylinders with radius  $R$



**Fig. 1.** Scheme of nano-patterned semiconductor–electrolyte interface: (a) top view showing negatively charged circular spots with  $R=30$  nm and  $L=100$  nm, and (b) side view showing negative charges at the spots and positive image charges located symmetrically with respect to the Helmholtz plane (dotted line).

and height  $h$ . Despite the simple form of such samples, the analysis of the corresponding potential profile is not straightforward, because there are a few different length scales ( $L$ ,  $R$ ,  $h$ , the depletion length in the semiconductor, and the length scale characterizing the double layer in the electrolyte) and different permittivities. For our present goals, we focus on one of the cases allowing nearly analytical analysis. In particular, we consider that the cylindrically shaped discs are thin,  $h \ll R$ , and treat them as circular spots, i.e., neglect their thickness. In this case, there are only two permittivities characterizing the electrolyte and semiconductor. We consider that the difference between these permittivities is minor and set them equal,  $\epsilon_1 = \epsilon_2 \equiv \epsilon$ . In reality, this situation takes place, e.g., in the case of  $\text{TiO}_2$  (the  $\text{TiO}_2$  permittivity is close to that of water, which in turn close to those of various electrolytes).

To calculate the electric potential, we should specify the charge distribution in different areas. Inside the semiconductor, the charge is located in the depletion zone. As already noted, this region is customarily described by using the Schottky model. The change of the corresponding potential can be appreciable. The thickness of this zone is, however, usually large, and the surface charge compensating the depleted charge is relatively small. In addition, the potentials related to the charge depletion and the charge on the circular areas are additive. Taking also into account that the features of the former (Schottky) potential are well known from textbooks, we exclude it from our analysis. The surface charge located outside the circular spots is considered to be small compared to that located inside and accordingly is neglected. The attention is focused on the potential related to the charge located inside the spots and the corresponding charge in electrolyte. The former charge is considered to be distributed there (at spots) uniformly.

To describe the screening of the charge located inside the circular spots, we consider that the electrolyte is strong and adopt the simplest Helmholtz model of the double layer. The standard version of this model implies that the interface is fully uniform and the surface charge is screened by the charge located in the electrolyte at distance  $l$ . The signs of these two charges are considered to be different while the densities are equal. Physically, this means that the region with  $0 < z < l$  is treated as a dielectric while the region with  $z \geq l$  is treated as a perfect conductor ( $z$  is here the coordinate in the direction perpendicular to the interface, and  $z=0$  corresponds to the interface). In our case, the simplest modification of this model might be to consider that the charge in the electrolyte is uniformly located at the circularly shaped areas located at a distance  $l$  from the charged spots at the interface. In this case, the potential at  $z=l$  would, however, depend on two other coordinates. This does not correspond to the treatment of the region at  $z \geq l$  as a perfect conductor. If we accept this treatment, the potential at  $z < l$  can be calculated by using the conventional method of image charges [9]. Following this line, we introduce the image charge located at a distance  $2l$  from the charged areas at the interface, as shown in Fig. 1(b).

With the specification above, the electric potential is determined in general as

$$\varphi(\mathbf{r}) = \frac{1}{\epsilon} \int \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} dV, \quad (1)$$

where  $\rho$  is the charge density (including the image charge),  $\mathbf{r}$  is the coordinate, and  $dV$  is a volume element. In our model, the charge is located on the surfaces, and accordingly the integration is performed in fact over the surfaces. For the geometry under consideration [Fig. 1], this integral can easily be calculated numerically. Analytically, one can obtain

$$\varphi = 0 \quad \text{at } z = l. \quad (2)$$

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