

# Quantum mechanical state of the quantum system, and tunneling effect (a new approach)

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**Abstract.** A physical model proposed in this paper resolves existing contradictions between wave and corpuscle properties of quantum particles (electrons) in tunneling effect. By means of AFM methods the work shows that the existence of the second electron on the other side of potential barrier is necessary to realize a tunneling effect in a probe-surface system. At this, only quantum mechanical state of the electron — not its corpuscular properties — described by the wave function tunnels (penetrates) through the potential barrier. The presence of the second electron on the other side of the potential barrier is necessary to establish concatenation with the first, so to say, ‘tunneling’ one. At lack of the second electron on the other side of the potential barrier, only tunneling quantum mechanical state of the first electron is possible — without transferring its corpuscular properties.

## 1 Introduction

At present time, the observation of tunneling effects in quantum systems with potential barrier is usually limited to metering electron (tunneling) currents flowing through such systems. The argument in its favor, for example, is the Nobel Prize for Physics awarded to David Josephson “for his theoretical predictions of the properties of a supercurrent through a tunnel barrier” in 1973. Up to now nobody observed the very process of electron penetration through the tunnel-transparent potential barrier.

It seems probable that the one of the reasons for it is contradictions associated with the wave-corpuscular nature of elementary particles — electrons in particular. Thus, along with the existing fundamental principles of quantum mechanics (energy and momentum quantization, Heisenberg uncertainty principle, Pauli exclusion principle, principle of identical particles), there are, so to say, concomitant auxiliary principles which up to recent times had no final definitions but played an important role in result interpretation in each individual quantum mechanical case. The examples of these auxiliary (non-fundamental) principles are: the inseparability of wave and corpuscular properties of quantum particles, the principle of locality (close-range action or discreteness of systems), the limitation of the quantum systems concatenation rate by speed of light.

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Thus, from the principle of inseparability of wave and corpuscular properties it follows that in tunneling effects corpuscular properties of quantum particle penetrate through the potential barrier together with its wave properties, i. e. they can present inside the potential barrier in the region of forbidden energy values. At this, in the light of formalism of the Schrödinger equation, in the barrier region the quantum particle is not described by the wave process at all, and outside the barrier region the oscillation properties are peculiar only to the wave function  $\Psi$  having no physical sense — only squared absolute value  $|\Psi|^2$  has one. On the contrary, in Klein paradox, within the solutions of Dirac and Klein-Gordon equations, the wave function keeps oscillations even at negative energies. Therefore, the wave properties of the electron, on the one hand, don't feature the full web of attributes of oscillatory system, but, on the other hand, have some specific peculiarities — coherent and non-coherent superposition, quantum entanglement — which are intrinsic to quantum systems only.

In addition to the stated above, the methodological violations at tunneling time definition (definition of the pattern of interaction with the barrier), coming from the measurement of various quantum processes in the same Kolmogorov probability space (with the use of the same detector), lead to the violation of causal relationship between the transmitted and the reflected wave packets, that resulted in its time in seeming (based on interference) exceedance of light speed in the processes of tunneling through the wide potential barriers, and occurrence of Hartman paradox.

The investigations of quantum teleportation effect, carried out at current technological level [1], disprove the principle of quantum system locality and establish the truth of the new principle of long-range action or discreteness of quantum systems (Bell's inequalities, entangled states), that proves (according to the no-cloning theorem for quantum objects, it is impossible to create the second identical copy of quantum state without killing the first one) discreteness of wave and corpuscular properties of the quantum particle.

At the same time, the investigations of quantum interference and quantum entanglement (concatenated states) [2] overcome a "light speed" limitation of the interaction establishment maximum rate.

The application of the individual Kolmogorov probability space for each measurement subprocess (using of several detectors) gives the opportunity to overcome methodological contradictions in determination of causal relationship in interaction of the transmitted and the reflected wave packets and the potential barrier, and resolve the Hartman paradox [3].

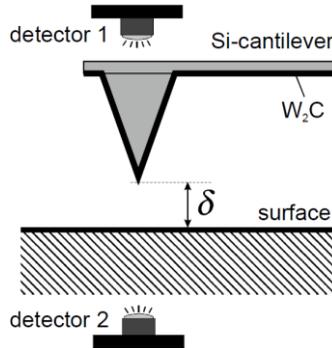
However, as it follows from the stated above, the existing amount of experimental data is not yet sufficient for complete realization of physical capabilities of quantum nanosystems, which is explained by the presence of unresolved contradictions associated with the wave-corpuscle duality of the elementary particle properties, which often manifest themselves in individual quantum-mechanical applications, e. g. in tunneling effects.

## 2 Study objects and experimental technique

According to [3], for the proper investigation of tunneling effect in case of one-dimensional complete scattering, it is necessary to use the individual Kolmogorov probability space — or individual detector — to describe (to measure the parameters of) each subprocess of transmitting and reflecting wave packet. For this purpose it is convenient to employ atomic-force microscopy (AFM) methods which give an opportunity to realize the proposed approach to the measurement of quantum-mechanical systems with the use of two detectors. For example, at the grounded wafer the first detector can be represented by the cantilever needle point (hereinafter referred to as a probe). And vice versa, at the grounded cantilever the second detector can be represented by the wafer (Fig. 1). Besides that, the AFM makes it possible to investigate local non-complete

scattering processes, which means measuring the tunneling parameters at the close proximity to the barrier.

To investigate tunneling effect in quantum-mechanical probe-surface system the SOLVER-HV high-vacuum AFM in semi-contact scan mode at resolution of  $N=256$  points in horizontal and vertical sweeps was used together with the application of Kelvin probe double-pass technique [4]. For this purpose, at the areas of  $50 \times 50 \text{ um}^2$  of conducting (n-n<sup>+</sup>-Si{111}) and non-conducting (thermal oxide SiO<sub>2</sub>/n-n<sup>+</sup>-Si{111}) surfaces the local  $10 \times 10 \text{ um}^2$  areas with positive Q<sup>+</sup> and negative Q<sup>-</sup> electric charge were formed. The concentration of electrically charged shallow-level donor impurities  $N_{D^+}$  in epitaxial n-layer of the n-n<sup>+</sup>-Si{111} structure was equal to  $\approx 10^{15} \text{ cm}^{-3}$ .



**Fig. 1.** The schematic illustration of the probe-surface system with the tunnel-transparent gap  $\delta$ .

To create electric charge at local  $10 \times 10 \text{ um}^2$  areas of the surface, during the scanning the electric bias  $U_p$  of the desired polarity was applied between the conducting cantilever needle point HA-HR/W<sub>2</sub>C and conducting semiconductor (n-n<sup>+</sup>-Si{111}) or non-conducting dielectric (thermal oxide SiO<sub>2</sub>/n-n<sup>+</sup>-Si{111}) surfaces. There were two cases to consider. In the first one, the bias  $U_p$  was applied to the immediate contact of the conducting cantilever needle point and the surface. In the second case, it was applied to the tunnel-transparent gap  $\delta < 10 \text{ nm}$  between them. In order to provide a good electric contact, at the reverse side of the structure — at the side of n<sup>+</sup>-Si(111) layer — a low-resistivity ohmic contact was formed by NiAu plating. The cantilever needle point HA-HR/W<sub>2</sub>C with the rounding radius  $r \approx 30 \text{ nm}$  was plated by conducting tungsten carbide W<sub>2</sub>C with the work function of  $\approx 4.9 \text{ eV}$ .

The contact electrostatic potential difference (CPD, hereinafter also referred to as a potential)  $\Delta\varphi(x,y)$  of the surface area under investigation was measured at the second pass of the AFM Kelvin probe technique with the use of the following expression:

$$\Delta\varphi(x, y) = \varphi_p - \varphi_S(x, y), \quad (1)$$

where  $\varphi_p$  is a surface potential of the probe needle point plating ( $p$  for probe), and  $\varphi_S$  is a studied surface potential ( $S$  for surface). Therefore, knowing the work function of the cantilever needle point ( $q\varphi_p$ ), from the expression (1) it is plain to find out potential  $\varphi_S$  (work function  $q\varphi_s$ ) of the studied area of semiconductor (n-Si(111)) or dielectric (SiO<sub>2</sub>) surface.

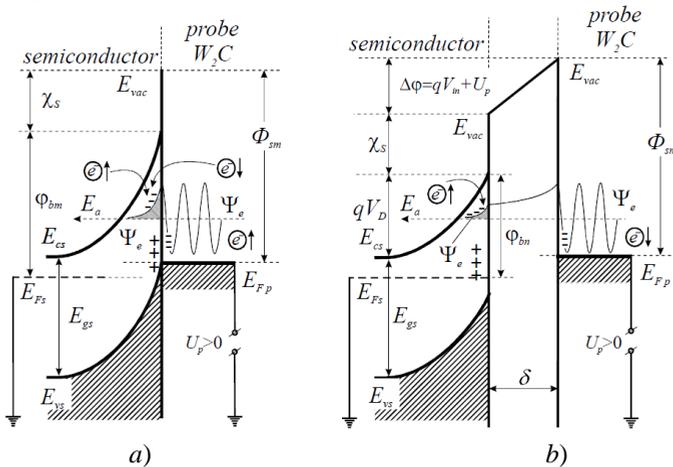
To reveal the effects, at first we estimated the distribution of electrostatic potential  $\Delta\varphi(x,y)$  (CPD) of clear (initial)  $50 \times 50 \text{ um}^2$  areas of semiconductor ( $q\varphi_s(\text{n-Si}(111)) \approx 4.12 \text{ eV}$ ) and dielectric ( $q\varphi_s(\text{SiO}_2) \approx 4.00 \text{ eV}$ ) surfaces. Then, at the same areas we carried out scanning of smaller  $10 \times 10 \text{ um}^2$  local areas with the application of external bias to the immediate contact between the probe and the surface, or to the tunnel-transparent gap  $\delta$  between them. After that, the one more scanning of the studied  $50 \times 50 \text{ um}^2$  areas was

carried out to reveal changes of surface electrostatic potential of local  $10 \times 10 \text{ nm}^2$  areas and to find out the polarity of their electric charges.

In accordance with the energy diagrams of the probe-semiconductor system — in the case of semiconductor structure grounding (Fig. 2, semiconductor-probe- $W_2C$ ) — and the probe-dielectric system (Fig. 3, insulator-probe- $W_2C$ ), the detector is represented by the cantilever needle point 'probe- $W_2C$ ' which gives an opportunity to register at the opposite side of the barrier with the thickness  $\delta$  the electron presence or absence judging by the change of surface electrostatic potential. If the bias is positive  $U_p > 0$ , the needle point has negative electric charge  $Q^-$ ; if the bias is negative  $U_p < 0$ , the electric charge is positive  $Q^+$  [6].

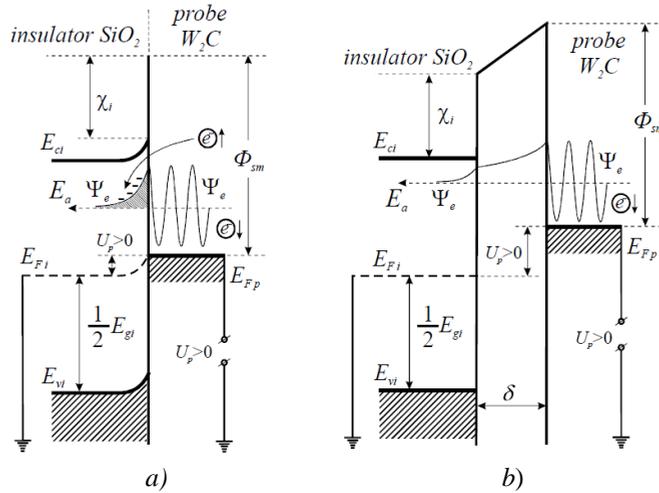
### 3 Experimental results

In case of the immediate contact between the cantilever needle point and both conducting semiconductor (Fig. 2,a) and non-conducting dielectric (Fig. 3,a) surfaces, it is possible to observe that positive bias  $U_p > 0$  application to the local  $10 \times 10 \text{ nm}^2$  surface areas leads to stable in time increase of CPD and decrease of work function ( $q\phi_s \approx 4.05 \text{ eV}$ ) — for the silicon; and stable in time decrease of CPD and increase of work function ( $q\phi_s \approx 4.16 \text{ eV}$ ) — for  $\text{SiO}_2$ . Such CPD changes go along with the occurrence of sufficiently stable in time negative electric charges  $Q^-$  on both local areas (Fig. 4,a and Fig. 4,b, the arrow 1).



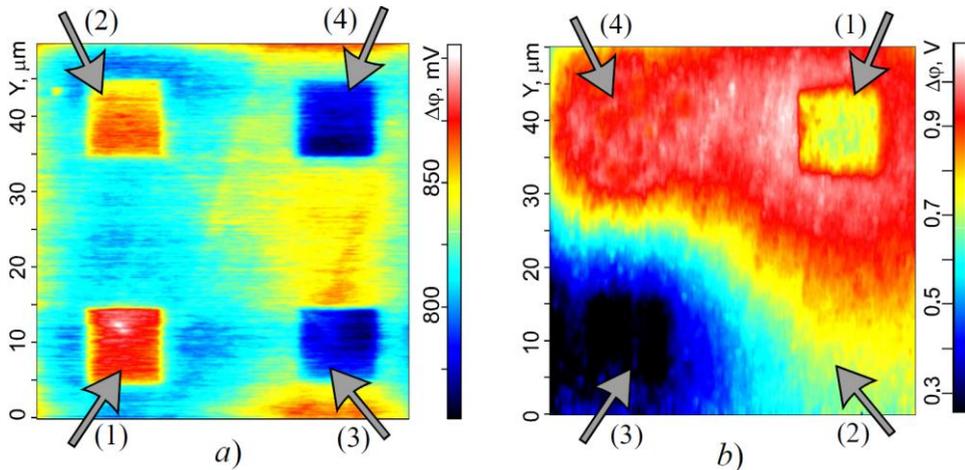
**Fig. 2.** The energy diagrams of the probe-semiconductor system with the grounded sample (structure) and application of positive bias  $U_p > 0$ : a) to the immediate contact of the probe and semiconductor, b) to the tunnel-transparent gap  $\delta \approx 10 \text{ nm}$  between them.

The observed allocation of negative electric charges (electrons) on the surfaces can be explained by the following considerations. Quantum-mechanical states  $\Psi_e$  of the electrons of the probe plated needle point, tunneling into the semiconductor or dielectric subsurface area, induce there the acceptor-type metal-induced states (the analogue of metal-induced states at the subsurface area of semiconductor in Schottky contacts [5]). These states form an array of deep acceptor levels  $E_a$  in the forbidden region, which are capable to capture free electrons at normal temperature, creating negative electric charge in local areas. In the case of the contact between the probe and semiconductor surface, such a charge can be created by both the own conduction electrons and conduction electrons diffusing from the cantilever plated needle point (Fig. 2,a). In the case of the contact between the probe and dielectric surface, such a charge can be formed only by the electrons diffusing from the cantilever plated needle point (Fig. 3,a).



**Fig. 3.** The energy diagrams of the probe-dielectric system with the grounded sample (structure) and application of positive bias  $U_p > 0$ : a) to the immediate contact of the probe and dielectric, b) to the tunnel-transparent gap  $\delta \approx 10$  nm between them.

In the same way, the negative bias  $U_p < 0$  probably leads to forming arrays of deep donor levels  $E_d$  in the forbidden region of the semiconductor or dielectric subsurface areas —  $q\phi_s(\text{n-Si}(111)) \approx 4.26$  eV for semiconductor,  $q\phi_s(\text{SiO}_2) \approx 4.63$  eV for dielectric — which are capable to capture holes in local  $10 \times 10 \text{ um}^2$  areas (arrow 3 in Fig. 4, a and 4, b).



**Fig. 4.** The AFM electrostatic potential image for the  $50 \times 50 \text{ um}^2$  area of semiconductor n-Si{111} — a) and dielectric  $\text{SiO}_2$  — b) surfaces. The arrows 1 and 2 point at the negative electric charge regions of the local  $10 \times 10 \text{ um}^2$  areas, the arrows 3 and 4 point at the ones of positive electric charge. The arrows 1 and 3 correspond to the areas charged through the immediate contact between the probe and the surface. The arrows 2 and 4 correspond to the ones charged through the tunnel-transparent gap.

It should be noted that the equal signs of the electric charges of the cantilever needle and the charged areas of the surfaces virtually eliminate the effect of mirror image forces.

The other situation is observed when there is a tunnel-transparent gap  $\delta$  in the probe-surface system (between the cantilever needle and the surface).

In this case, the negative (Fig. 4,*a*, arrow 2) and the positive (Fig. 4,*a*, arrow 4) electric charges can be created only on the conducting semiconductor surface n-Si. Here, the electric charges on semiconductor surface can be created by the own mobile electrons and holes occupying vacant donor  $E_d$  and acceptor  $E_a$  metal-induced states  $\Psi_e$  in subsurface semiconductor area, which are formed by electron  $\Psi_e$  (Fig. 2,*b*) and hole  $\Psi_h$  states tunneling from the plated cantilever needle point. The fact that it can be only own semiconductor charge carriers is proved by the same experiments with dielectric surface, described below.

The absence of the own mobile electric charge carriers (electrons and holes) on the surface and in subsurface area of the dielectric makes the creation of negative (Fig. 4,*b*, arrow 2) or positive (Fig. 4,*b*, arrow 4) electric charge there impossible, in spite of tunneling of electron  $\Psi_e$  and hole  $\Psi_h$  states into subsurface area, even at presence of smaller  $\delta < 10$  nm tunnel-transparent gap. This fact can be explained by the following: due to the absence of free electric charge carriers, metal-induced states  $\Psi_e$  and  $\Psi_h$  formed by electron  $\Psi_e$  and hole  $\Psi_h$  states tunneling to the dielectric subsurface area stay vacant, and the creation of stable electric charges on them does not take place (Fig. 3,*b*).

According to the Pauli principle, in order to occupy the metal-induced state in semiconductor subsurface area the electron must have a spin opposite to the one of the electron localized on the other side of the barrier. At this, such electrons can form concatenated quantum states.

The same transferring quantum states of electrons  $\Psi_e$  and holes  $\Psi_h$  in tunneling effects without transferring their corpuscular properties is also observed for dielectric Ta<sub>2</sub>O<sub>5</sub> and Si<sub>3</sub>N<sub>x</sub> surfaces.

## 4 Conclusions

The independence of wave and corpuscular properties of quantum particles on each other gives the opportunity to take a new look at tunneling effect in probe-surface system in the AFM method in terms of tunneling only their quantum-mechanical states.

The quantum-mechanical states of the electrons  $\Psi_e$  and holes  $\Psi_h$  tunneling from the cantilever plated needle through the potential barrier (the gap between probe and surface) induce metal-induced states in semiconductor or dielectric forbidden region, which are identical to those induced in semiconductor of Schottky contacts.

In order to create electric charge on the surface through the tunnel-transparent gap, it is necessary to have mobile electric charge carriers on it. This idea is proven by the experiments with dielectric surfaces.

The absence of mobile electrons and holes in dielectric at the opposite side of the tunnel-transparent barrier (gap) points out that in given tunneling process the corpuscular properties of electrons and holes do not penetrate through the tunnel-transparent gap.

The proposed fresh look at quantum-mechanical tunneling effect — from the point of view of fundamental notions (of wave-corpuscular duality) — is necessary to build adequate physical models of quantum nanosystems which give a new way to describe unusual and paradoxical effects in quantum nanosystems. These effects may be used to increase stability of physical states of quantum computer cubits, sensitivity of quantum sensors, their controllability; make organization of interconnections between the elements of such systems more effective; enhance security of transmission lines; improve quantum state transferring processes not only between the identical quantum objects but between the objects of different physical nature (e. g. between quantum particle and transmission line); advance discrete quantum devices; develop and design high-performance quantum nanocomputers on the basis of semiconductor nanotechnologies.

The identical effects are also observed for n-GaAs and n-GaN surfaces.

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