Phenomenological model of an abnormal thermal field electron emission from the 2D nanoheterostructured surfaces

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Abstract Phenomenological model of an abnormal thermal field electron emission from the 2D nanoheterostructures of a kind: a conductor – a thin dielectric film, is offered and developed.

1. Introduction
As is known [1], a phenomenon of an excitation of a self sustaining electron emission from the thin oxide dielectric films was revealed and systematically investigated by Malter [1]. “Malter emission” is the electron emission from the thin high-resistivity materials films with the high-secondary-electron coefficients, induced by a primary electron beam directed at the film front surface [1, 2].

Now it is established that the basic features of the Malter emission phenomenon takes place for a wide range of the 2D nanoheterostructures (NHS) of a kind: a conductor- a thin dielectric films [1-5].

The basic features and laws of the Malter emission phenomenon\(^1\) or, other words, ATFE phenomenon consist in the following.
1. ATFE occurs for various NHS, formed by the thin (1 ÷ 10^4 nm) dielectric films (in particularly, A12O3 + Cs2O, MgO, B2O3, KCl, SiO2, CdS, ZrO2, diamond, diamond like, carbon and polymeric films) on the conducting substrates surfaces. ATFE process properties depend from the film formation technological conditions and its thickness, physical-chemical properties of the NHS substance, temperature and also of the film doping degree by the impurities.
2. For ATFE excitation it is necessary to "activate" emission process by an external physical impact at NHS substance (by electron or ion bombardment, NHS heating).
3. Emission process functional dependence \(I_e (F_e)\), where \(I_e\) is an emission current, \(F_e\) is the normal component extracting field strength, does not submit to field emission (FE) and thermal field emission (TFE) theories [2, 6].

\(^1\) Malter emission phenomenon we will name here as an abnormal thermal field emission (ATFE). In our opinion, the offered abbreviation more adequately and correctly reflects the basic features and anomalies of the low-macroscopic field (LMF) electron emission processes [2] activated impact on the NHS substance of various external physical factors.
4. ATFE phenomenon takes place for the NHS with various geometry and superficial morphology. In particular, ATFE it is observed as for NHS samples on a basis of tip-shaped wide band gap semiconductors and for 2D NHS on the basis of diamond like films, carbon films and also for carbon nanotubes [5].

5. $F_e$ numerical values necessary for activation and maintenance ATFE process approximately at 2-3 order is less than field strength necessary for field emitters on the homogeneous substances basis.

Listed ATFE properties and, in particularly, high NHS emission ability at rather low values $F_e$, represent considerable practical interest for realization of the some modern projects for vacuum microelectronics and also for high current electronics [2, 5].

However, despite rather long history of researches ATFE phenomenon has no adequate quantitative interpretation till now. The purpose of the present work consists in designing semi quantitative phenomenological model for ATFE phenomenon.

2. Phenomenological model of the ATFE phenomenon

The model of the ATFE phenomenon was constructed on the basis of generalization of the data obtained in the previous researches of thermal field emission properties of the low-dimensional NHS [1-5]. To create ATFE model a real vacuum diode was modeled by a 2D NHS placed into vacuum in a homogeneous electrostatic field $F_e$ (figure 1).

The model was based on following assumptions.
1. Electron injection from metal to dielectric through the metal-dielectric barrier, can involve both thermal field emission and thermionic emission (TE) mechanisms; the metal-dielectric junction is locking for metal electrons;
2. Electric field on the metal-dielectric interface is a superposition: of an external field ($F_e$), field of the positive space charge (SC) formed as a result of ionization of the localized states in the dielectric film band gap and also SC field of electrons injected into the dielectric conduction band;
3. Ionization of the localized states in the dielectric film band gap may occur both by thermal field mechanism and, generally speaking, under action of the electromagnetic radiation absorbed by the film, including thermal radiation of NHS substance;
4. At small thicknesses of the dielectric film (about the free path length of low-energy electrons in relation to the process of electron-phonon interaction) electron transport in the film is occurs mainly by the quasi-ballistic mechanism;
5. The electron flux emitted into vacuum was accepted to be equal to the product of probability of electron tunneling through the potential barrier on the dielectric–vacuum interface (in WKB approximation [6]) by the electron flux injected into dielectric.

The space charge density distribution ($\rho$) formed in a result of ionization of the localized states in the band gap of the dielectric film, was approximated by the function

$$\rho = \rho_0 \exp \left[ -x^2/(\lambda^2 \tau^2) \right],$$

where $x$ ($x \leq \tau$) is the coordinate counted from the metal – dielectric interface in a direction to the dielectric-vacuum interface; $\tau$ is the dielectric film thickness; $\lambda$ is a dimensionless parameter; $\rho_0 = qN_t/\varepsilon \varepsilon_0$, here $q$ is an absolute value of the electron charge; $N_t$ is the density of the ionized localized states; $\varepsilon$ is the dielectric film permittivity, $\varepsilon_0$ is an electric constant.

The Poisson equation solution for the potential distribution $\varphi(x)$ in the film with boundary conditions

$$\varphi \bigg|_{x=0} = 0; \quad \left. \frac{d \varphi}{dx} \right|_{x=\tau-0} = \frac{F_e}{\varepsilon},$$
where $F_e$ is the absolute value of the field strength on the dielectric-vacuum interface (at $x = \tau + 0$), looks like

$$\varphi(x) = \frac{F_e}{\varepsilon} x + \frac{\sqrt{\pi} \lambda \rho_0}{2} \text{erf}\left(\frac{x}{\lambda}\right) x + \lambda^2 x^2 \rho_0 \frac{1}{2} \left[1 - \left(\frac{x}{\lambda} \text{erf}\left(\frac{x}{\lambda}\right) + \exp\left(-\frac{x^2}{\lambda^2 x^2}\right)\right)\right]$$

(2)

Figure 1. Two barrier energy band diagram for ATFE phenomenon modeling

Note that equation (2) describes the potential distribution $\varphi(x)$ in the so-called "zero current" approximation. This approximation is valid when the inequality $N_t >> n_e$ holds, here $n_e$ is a concentration of the electrons injected into the dielectric film.

The current densities of electrons injected from the metal into the film by the thermal field emission ($J_{TJE}$) mechanism of and by the thermionic emission mechanism ($J_{TE}$) above the Schottky barrier can be described by the following expressions [7]

$$J_{TJE} = A^* T_s^2 \left(\frac{\pi e^{00}}{k^2 T_s^2}\right)^{\frac{1}{2}} \left[q \varphi_s + \frac{\phi_b}{\sqrt{\frac{e^{00} E_s}{c h^2 k T_s}}}ight]^{\frac{1}{2}} \times \exp\left(-\frac{\phi_b}{E_0}\right) \cdot \exp\left(\frac{q \varphi_s}{E_1}\right)$$

(3)

where $A^*$ is a constant which, generally speaking, depends on electron effective mass ($m^*$) and includes a quantum-mechanical factor of electron reflection from the interface, $T_s$ is the NHS material temperature, $\varphi_s$ is the surface potential of the film on the dielectric – vacuum interface,
\[ \phi_b = \phi_m - \chi \left( \frac{q^b \cdot (\phi_m - \phi_d + q \cdot \phi_d) \cdot N_t}{8\pi^2 e^3 \varepsilon_0^2} \right)^{\frac{1}{2}}, \]

here \( \phi_b \) is the potential barrier height at the metal-vacuum interface, \( \phi_m \) is the work function of an electron leaving the metal, \( \chi \) is the electronic affinity of the dielectric, \( \phi_d \) is the work function of an electron leaving the dielectric surface,

\[ E_{00} = \frac{qh}{4\pi} \left( \frac{N_t}{m^* \varepsilon \varepsilon_0} \right)^{\frac{1}{2}}, \]

\[ E_0 = E_{00} \cdot \text{cth} \left( \frac{E_{00}}{kT_s} \right), \]

\[ E_1 = E_{00} \cdot \left[ \text{th} \left( \frac{E_{00}}{kT_s} \right) \right]^{-1}, \]

where \( h \) is the Planck constant, \( k \) is the Boltzmann constant, \( m^* \) is the effective electron mass,

\[ J_{IE} = A^* \cdot T_s^2 \cdot \exp \left( -\frac{\phi_{d}^b}{kT_s} \right). \]  

The values \( N_t \) (\( T_s, F_e \)) were defined from the known semiconductor physics relations between the concentration of the ionized localized states, substance temperature and electric field strength.

To perform numerical calculations with equations (3) and (4), the initial parameters describing physicochemical and structural properties of modeled NHS were taken from the data of [8 - 16]. For carrying out of numerical calculations and estimations the concrete NHS was used, namely, ZrO2/W<100> needle-shaped microcrystal [17]. In view of these remarks, the calculations were carried out using the following set of parameters: \( \phi_m \approx 4.0\text{eV} \) (for W(111)); \( \phi_m \approx 4.5\text{eV} \) (for W(100)); \( \phi_d \approx 4.0\text{eV} \) (for ZrO2); \( m^* \approx 0.5m_e \); \( \chi \approx 3.0\text{eV} \) (for ZrO2); the thickness of a dielectric film was accepted equal to \( \tau \approx 10\text{nm} \); the density of non-ionized localized states \( (N_{0d}) \) in the ZrO2 film (from different sources [11 - 13]) can make up from \( 5.0 \times 10^{24} \text{m}^{-3} \) to \( 5.0 \times 10^{25} \text{m}^{-3} \); the maximum density of the localized states should be at a depth \( E_d \approx 0.8\text{eV} \) under a bottom of the ZrO2 conductivity band [10]; the average free path length of electrons in relation to electron-phonon interaction in various thin oxide films is from \( 3\text{nm} \) up to \( 100 \) (and more) nm. The probability of tunneling through dielectric-vacuum potential barrier for partly thermalized electrons was accepted equal to the transparency of the potential barrier calculated in the WKB - approximation [6].

Results of modeling are given on figure 2.

From the curves resulted in figure 2, in particular, it is easy to see that emission ability of ZrO2/W<100> NHS is significantly (~ 3-4 orders of magnitude) higher than for the Schottky-cathode (see figure 2; curves 1 and 2). In the area of rather low of external electric field intensities \( (F_e < 50\text{V/\mu m}) \) the emission flux from the surface of ZrO2/W<100> NHS is formed mainly by electrons injected into ZrO2 film as a result of thermionic (TE) process (and extended Schottky emission (SE) process) above the Schottky barrier from the surfaces of planes \( \{100\}, \{110\} \) and \( \{111\} \) of the W<100> microcrystal. At \( F_e \geq 100\text{V/\mu m} \) (when the transparency of the barrier becomes equal to \( \approx 1 \) (both for "TE", and for "TFE" injected electrons)) the emission current rather weakly depends on \( F_e \).
Figure 2. Emission current density versus field strength on the surface of ZrO2/W <100> NHS (experimental (curves 1, 2) [17] and modeling (curves 3-6) data)
1. T_s = 2000K; the thickness of ZrO2 layer is equal to one monolayer; 2. T_s = 2000K; the thickness of ZrO2 layer is equal to $\approx 5$nm; 3. For electrons injected into ZrO2 film from planes W{100} by the TE mechanism; 4. For electrons injected into ZrO2 film from planes W{100} by the TFE mechanism; 5. For electrons injected into ZrO2 film from planes W{111} by the TE mechanism; 6. For electrons injected into ZrO2 film from planes W{111} by the TFE mechanism.
(For curves 3 - 6: $T_s = 2000K; N_{00} \approx 10^{25}$m$^{-3}$; the thickness of ZrO2 layer is equal $\approx 5$nm)

3. Conclusions
The above-stated results, as it is represented, allow making the following conclusions.
1. The main factor, which defines the unusual features (or anomalies) of the ATFE process from the surface of the low-dimensional NHS, is formation of the high density bounded space charge on the localized states in the band gap of the thin dielectric film.
2. In the ATFE conditions the emitted in vacuum electron flux is formed by electrons injected into a dielectric film by the mechanism of TE (above Schottky barrier) and by the mechanism of TFE. In other words, the physical mechanism of ATFE is complex and is not reduced only to one of the known classical TE and TFE phenomena.
3. ATFE properties: super high emission ability and stability of process, rather low level of $F_e$ and also high density of an emission current (up to $10^8$A/cm$^2$ and more) can be used in different areas of micro - and nanoelectronics, including high power electronics for produce high-intensity stationary electron sources [5].
4. ZrO2/W and ZrO2/Mo NHSs does not seem to be unique in its physicochemical and structural properties. To form new NHS - effective ATFE electron sources (based both on 1D or 2D structures
and ordered ensembles NHS) having a priori given emission properties (in particular, capable of ATFE of high current density at $T = 300K$) additional special researches using methods of modeling layer-by-layer epitaxial thin dielectric film growth processes and also methods of "zone engineering" are necessary [18, 19].

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