Multiscale simulation of surface characteristics of field emitter tip

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Abstract. Paper presents multi-scale modelling of the field emitter tip surface characteristics. At micro-scale an approximation of emitter shape is obtained, at meso-scale crystallographic faces are constructed for application of a semi-empirical regression model of work function distribution, on the nano-scale surface atoms coordinates are calculated that serves as base data for all the above mentioned levels of detail. Electric field distribution at all scale levels is calculated.

1. Introduction
An important problem of using computational models for simulation the properties and characteristics of emission systems is accounting for multi-scale nature of the physical phenomena that occur during the process of field electron emission. One of the principal problems of multi-scale modeling is the need to conjoin a number of different models describing the behavior and properties of complex systems with different levels of detail.

A combination of classic and quantum approach in emission system modeling at different scales is an extraordinarily complex and currently topical problem. The solution for the problem of constructing a multi-scale models that would unite conceptually different algorithms for describing nanostructured system behavior on different levels in the hierarchy — i.e. on nano-, meso-, micro- and macro-scale — allows to conjoin the formulations for 1D-, 2D- and 3D-problems. The study gives the examples of such models and systems.

2. Simulation of structural, crystallographic, work function and electric field characteristics of field emitter tip surface
Multi-scale modeling is not only modeling on different scales (from subatomic to macro-level), but also on different levels, as the results for one level of scaling can be used like the input data for the next one. The object of study is a metal single crystal emitter tip made out of metal wires of diameters about 0.1−0.15 mm by the use of anode electric etching. The field emission phenomena occur with electric field strength of the order of $10^9−10^{11}$ V/m. Usually such fields are observed on surfaces of emitters with tip curvature radii of about 10−1000 nm. For example Figure 1 shows possible shapes approximating emitter as equipotential surfaces of the electric field [1] generated by charged cone with a sphere at the top (dotted line). As can be seen, the emitter apex shape is close to a hemisphere.

One of the problems that require multi-scale approach is the problem of computing the electric field above the emission surface. This is caused by the direct influence on the result by both nano- and micro- (atom packing density distribution, work function values, local surface curvature radius etc. [2−7]) and macroparameters (geometry of the electrode systems which defines the distribution of the macroscopic electric field).
Figure 1. Models hierarchy chart: shape approximation of emitter; construction of a set of coordinates of surface atoms, localization of crystallographic faces (the model structure of the apex surface, where the surface layers of the atoms of different depths of 0.2, 0.4, 0.6 and 0.8 lattice parameters and Miller indices for major crystal faces are represented); calculation of work function map, local electric field vectors over surface atoms (calculated by the finite-differences method) and simulated pattern of field electron emission.

The number of the detalization levels of different scales during modeling depends on the complexity of shape and structure of the emitter. Those levels can also be categorized by the three principal functions that are simultaneously performed by the electric field in field emission systems: generation, acceleration and transportation. Field electron current is generated in process of emission on the nanoscale: under the influence of the field the surface threshold turns into a potential barrier which can be tunneled through with a non-zero probability, as described by the quantum theory. The electric field strength which causes the width of the potential barrier to be in order of nanometers, is formed due to the presence of nanostructure details of the surface and due to amplification of the
larger scale field. Hence, this level of modeling is donned nanoscale. The most important problem of modeling on nanoscale is defining the exact maximum distance to the surface on which the nanoscale defects have any significant impact, and computing the field enhancement coefficient.

On the microscale the field distribution is defined by microscale geometric parameters of field emission systems. The non-uniform distribution of surface work function values causes patch field effect due to contact potential difference established between areas having different work function values.

On the macroscale the field emission electrode systems usually corresponds to a calculation area of complex shape which includes the boundaries of the emitter with large surface curvature and small size, the fact that leads to a rather large range of the characteristic sizes in the same geometric configuration. Moreover, the exponential dependence of the field emission current density [8] requires increased precision for taking into account the emitter’s boundary conditions:

\[
J(F) = e^3 / \left( 8 \pi \varepsilon_0 F^2 \right) \exp \left( \frac{8 \pi (2m)^{1/2}}{3 \hbar \Phi} \right) \left( \frac{y}{F} \right)^{3/2} \nu(y),
\]

where \( m \) and \( e \) are electron mass and charge, \( h \) is Planck’s constant, \( \Phi \) is the work function, \( F \) is the electric field strength, \( r(y_0) \) and \( \nu(y_0) \) are Nordheim’s elliptic functions, which can be approximated as [9]

\[
\nu(y) \approx 1 + y^2 (\ln y - 3)/3, \quad r(y) \approx 1 + y^2 (1 - \ln y)/9.
\]

The microscale electric field’s distribution near the emitter surface can be calculated analytically by the sphere-on-cone model [1]. Within the framework of this model one equipotential surface (Figure 1) of the electric field created by the charged orthogonal cone with the sphere at the top is taken as the emitter and the other one, as the anode. The electric field strength is given by the expression

\[
F_{\text{micro}} = V_R \left( m \cos \theta + (n + 1) a^{2n+1} r^{n-1} \right) \left( P_n(\cos \theta) \right)^2 / R^{2n} r^2 + \left( a^{2n+1} r^{n-1} - r^n \right) (n+1)^2 \left( \cos \theta P_n(\cos \theta) - P_{n+1}(\cos \theta) \right)^2 / R^{2n} r^2 \sin^2 \theta \right)^{1/2},
\]

where \( V_R \) and \( R \) are the anode voltage and anode distance; the shape of the anode is approximated by

\[
r \approx R / P_n(\cos \theta)^{1/n},
\]

\( a \) is the sphere radius; \( P_n \) is the Legendre function of the first kind of \( n \)th order given by the expression

\[
P_n(\cos \theta) = \frac{2}{\pi} \left[ \int_0^\theta \cos \left( n + \frac{1}{2} \right) x / \left( 2(\cos x - \cos \theta) \right)^{1/2} dx \right]
\]

and \( n \) is determined from the condition \( P_n(\cos \theta_0) = 0 \). On the surface of cone and sphere there is the condition \( V = 0 \).

In this approach one has to compute local values of the work function for various crystallographic planes of the emitter tip, using either ab initio calculation methods or empirical models [10, 11]. Figure 1 shows the hierarchy chart of models and their relations useful for understanding and development of the theory and relating it to experimental data.

3. Conclusion

This study presents the mathematical atomistic model of characteristics of emitter surface that is the study object of atom probe tomography, field emission electron/ion microscopy and field desorption microscopy, where crystallographic, work function and electric field characteristics of field emitter tip surface are of great importance [12].

In order to achieve a more in-depth understanding of the existing monocrystalline emitters, and to develop them further it is necessary to study further, considering both macroscopic processes (electric field distribution in the interelectrode gap; formation of the spatial charge) and microscopic parameters (formation and deformation of crystallographic faces, distribution of atomic packing...
density and of work function). Such a combined approach to the processes with temporal and spatial scales being that different is only possible using multiscale computer modeling.

Acknowledgments
Scientific research were performed at the Research park of St. Petersburg State University Computing Center.

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