Modelling of field emitter surface structure

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Abstract. The paper presents a mathematical model of the crystal structure of the emitter, which is the subject of research in atom probe tomography and in the field electron microscopy. Electronic, mechanical and other properties of the sample having the shape of the tip with a radius of curvature at the top of the order of hundred nanometers, these methods are considered on the basis of field desorption and emission (electron or ion). Strong electric field simultaneously performs generating, focusing, accelerating and transport function. Therefore, multi-scale modeling of the properties of the sample, including an approximation of its shape on the micro-, meso- and nanolevel, calculation of atomic packing density and size of crystal faces is a topical applications and is used to interpret the results of field emission experiment.

1. Introduction
Field emission properties of crystals are depended on surface structure. Information about the processes that occur on the metal surface in conditions of influence of strong electric fields, are important from the practical point of view for technologies of manufacture and use of electron and ion emitters, atom probes, field emission and scanning electron microscopy. Studying those phenomena is also useful for theoretical science [1−17] as it allows to obtain the data of mechanisms and properties of diffusion processes, crystal growth, self-organization and phase transitions, to measure such values as surface tension (free surface energy) in solids, energies of interaction of atoms and molecules with the surface and between each other.

The object of study is a metal single crystal emitter tip, which can be made out of metal wires of diameters about 0.1−0.15 mm by the use of anode electric etching.

Emission properties of crystal substances are in a great extent defined by the electron work function. It is usually assumed that this value has both surface and volume parts. Most probably, both of them have a non-negligible influence. The impact of the surface structure can be observed in the fact that faces with different Miller indexes have different work function values. But it's the volume that supplies the electrons to the surface and it's unacceptable to neglect this.

The goal of this research is development of model for surface structure of field emitter, based on its meso-scale shape approximation and atomistic calculation of crystal lattice inside this shape. Subproblem of this modeling is work function map calculation for the surface of emitter.

2. Surface structure calculation
Calculation of the atomic structure of the surface of monocystal emitter tip is a basic step in many models of both electron and ion field emission. As the emission properties are mostly defined by
relatively thin layer below the surface, it is only necessary to take in account the coordinates of atoms that lie up to certain depth and store them in computer memory. The surface atoms are defined as ones having an incomplete set of neighbors of a certain order, which distinguish them from the atoms in volume.

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 hemisphere. The model structure of the apex surface is shown in Figure 1c and 1d, where the surface layers of the atoms of different depths (0.2 and 0.4 lattice parameters) and Miller indices for major crystal faces are represented. The model structure of the apex surface is shown in Figure 2, where the surface layers of the atoms of different depths (0.2 and 0.4 lattice parameters) and Miller indices for major crystal faces are represented. Computational algorithm is based on [2, 3] and implemented in the Matlab environment.

![Figure 1](image1.png)
**Figure 1.** Emitter profile and shape approximation.

![Figure 2](image2.png)
**Figure 2.** Apex surface structure models with depth 0.2 and 0.4 lattice parameters.
Figure 3. Apex surface structure models with depth 0.6 and 0.8 lattice parameters.

Figure 3 shows surface layer with depth 0.6 lattice parameters, where 5160 atoms (highlighted) have full set of first order neighbours and 0.8 lattice parameters, where only 838 atoms (highlighted) have broken bounds with nearest neighbours of first order.

3. Work function surface map

Although, in principle, work function can be calculated directly (by the DFT method and the cluster model of the surface, but it is practically difficult to implement for whole surface, because of the large numbers of atoms on the surface. Another approach is more practical, although it does not take into account effects such as relaxation and reconstruction of the surface, but also requires an analysis of the coordination numbers that characterize the types of atoms (step, kink, with different binding energy and different local values of the work function.

The results of paper [18] show that the semiempirical model proposed by Surma can be used successfully to predict metal work functions near the crystal faces, experimental data on which are lacking, for example, in the simulation of the phenomenon of field electron emission. The error of such a prediction can be at a level of 0.2 eV. It is important to mention that, in tested cases of tungsten, molybdenum, platinum and iridium the Surma model was assumed to be statistically significant [18].

In this paper work function simulation is based on Surma model and this aspect is new for field emitter surface structure model, applicable to field electron/ion microscopy simulation, as well as for field desorption microscopy and atom probe tomography [4].

The simulation of the work function values nonuniform distribution (due to crystallographic anisotropy) over the surface of the emitter is carried out within the framework of the broken-bounds approach. Figure 4 shows work function map of the emitter surface.
Figure 4. Model map of work function distribution over the tungsten emitter surface (one quarter of the hemispherical apex of emitter).

4. Conclusion
The developed mathematical model describes the surface structure of the field emitter metal tip taking into account the arrangement of different crystallographic faces at the top of the emitter. This study can be associated with the model of patch field effect due to contact potential difference established between areas having different work function values.

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