Modelling of field desorption of monocrystal nanotip

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Abstract. Mathematical and computer model of field desorption process from metal nanocrystal tip is proposed. The radius of curvature on the top of the emitter is about 50 lattice parameters. The model includes initial calculation of intersection between the crystal lattice and emitter shape for bcc and fcc crystal structures. Arbitrary axisymmetric shapes (figures of rotation) can be used for the emitter model. The algorithm for allocation of atoms being desorbed at given time step is based on an analysis of geometric environment with specified local electric field. Polyhedron nanostructured shape of emitter is obtained as result of evaporation. Computer program realization (Matlab stand alone application) is presented.

1. Introduction

The object of this study is a tip-shaped metal field emitter with a monocrystal on its top. The main goal is constructing a model of structure of emitter surface under influence of an electric field at given temperature. Field desorption can lead to a particular surface structure that does not depend on the starting shape of the emitter but characterizes the lattice type and size of the monocrystal. This fact can probably be used for further determining of emission experiment conditions and corresponding models of both electron [1-12] and ion [13] field emission. As such, this study is of interest for such fields as field desorption microscopy and atomic probe tomography, that are among the modern methods of studying of 3d structure in solid bodies [14].

In accordance with this goal the following problems have to be solved: detection of the outline of the experimental sample emitter tip on a microphoto and finding the coordinates of its cross-section points using the Sobel operator; choosing a second-order rotary surface that would be the best approximation for the emitter shape using the method of the least squares; finding an equidistant line for the forming surface for modeling thin subsurface layer using the method of bisection; calculation of atomic structure of emitter tip surface based on the chosen approximating shape and crystal lattice type; choosing a model criterion of field desorption from the emitter surface and construction of corresponding model algorithm that would satisfy the desorption criteria; implementation of this algorithm and computation of emitter surface structure under the influence of temperature and electric field. This paper focuses on the latter two of those problems. The preceding ones are in greater detail considered in [2].


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2. Simulation algorithm for field desorption process

For a given value of the electric field strength on the surface of the monocrystal nanotip the most protruding atoms evaporate firstly, as having the highest number of broken bonds with neighboring atoms of the crystal lattice.

In [1, 2, 13] it was been shown that without a substantial loss of accuracy, we can confine ourselves to the fifth order of nearest neighbors in the analysis of crystallographic faces on the surface of the emitter tip. Therefore, analysis of the number of broken bonds in this paper was carried out with the same view of the nearest neighbors up to the 5-th order.

We used the method described in [15] to take into the atomic environment to simulate the field evaporation of the crystals.

For the atoms with the fewest nearest neighbors following characteristics have to be calculated: attributed coordination number N_{attr}, characterizing the binding energy of the atom with a given environment on the sample surface; the binding energy E; the average evaporation time Δt_m by the following expressions (1)−(4).

$$N_{\text{attr}} = \sum_{i=1}^{5} N_i k_i, \tag{1}$$

where N_i is the number of i-th order neighbors of an given atom, k_i is factor describing the dependence of the energy Ψ of pair interaction of atoms on the distance between them. In the simplified assumption that the interaction energy (binding energy) of an atom with its neighbors decreases in proportion to the sixth power of the distance [15]

$$k_i = g_i^6 g_1^{-6}, \tag{2}$$

where g_i is the distance to the i-th order neighbor.

Full binding energy of atom on the surface or in the volume of the crystal

$$E = \sum_{i=1}^{5} N_i \Psi_i = k_1 N_1 \Psi_1 + k_2 N_2 \Psi_1 + k_3 N_3 \Psi_1 + k_4 N_4 \Psi_1 + k_5 N_5 \Psi_1 = \Psi_1 \sum_{i=1}^{5} N_i k_i = N_{\text{attr}} \Psi_1, \tag{3}$$

where Ψ_i is the energy of pair interaction with i-th order neighbouring atom.

For selected atoms with the lowest binding energy E the evaporation time (can be interpreted as the mean value of the time during which an atom with a given environment stays on the surface in a bound state) was calculated

$$\Delta t_m = c \exp\left[10^4 \eta T^{-1} \left(c_1 F^{1/2} + c_2 N_{\text{attr}}\right)\right], \tag{4}$$

where η, c, c_1, c_2 are constants [15], T is the temperature; F is the electric field strength.

It specifies the time Δt of stable existence of corresponding configuration of the surface as the least evaporation time for all atoms with the lowest binding energy.

Simulation of the evaporation process at this stage is completed by removal of atoms, which have the evaporation time equal to Δt, and algorithm is repeated again for the new configuration of the nanotip by simulating the next stage of the process.

It is necessary to note that although in this approach the strength of field F can be calculated for each step of the algorithm taking into account the changing surface cross-section, in this research we used a constant value for F, which may be seen as a drawback. On the other hand, this algorithm takes in account the local neighborhood (i.e. number of neighbours) for each of the surface atoms and its changes during the desorption process. This is a positive side of the model.

3. Modeling results

Simulation algorithm was implemented in Matlab. Table 1 presents calculated data for tungsten monocrystal nanotip (bcc crystal structure, radius of apex curvature is 50 lattice parameters) characterizing the process of field desorption (field strength is 48 GV·m^{-1}, temperature 78 K).

Figure 1 shows the dependence of number of desorbed atoms on time of evaporation. The interesting result from figure 1 is that during desorption process an increasing number of atoms leaving the surface, it shows that evaporated emitter decreases with time taking the form of a polyhedron. One can suppose that the sides would be more smooth if local increases in electric field strength on particular areas of emitter surface were to be taken in account.

Figure 2 shows a model of a segment of a hemispherical apex of the emitter, formed as result of the process of field evaporation. Area of some crystal faces increased on the surface of the emitter comparing to the original form.

Table 1. Atomic environment (type of bond), values of N_{attr} and evaporation times Δt_m of atoms in several different configurations on the tungsten nanotip surface.

Coordination numbers $N_1 - N_2 - N_3 - N_4 - N_5$	N_{attr}	Δt_m (s)
4–3–6–11–3	5.91	$2.93 \cdot 10^{-8}$
4–3–6–12–3	5.93	$2.43 \cdot 10^{-7}$
4–4–6–12–4	6.38	$7.58 \cdot 10^{-3}$
6–3–7–12–4	8.00	$1.92 \cdot 10^{9}$
6–4–12–4–6	8.21	$3.96 \cdot 10^{11}$
6–4–7–14–6	8.51	$2.30 \cdot 10^{16}$

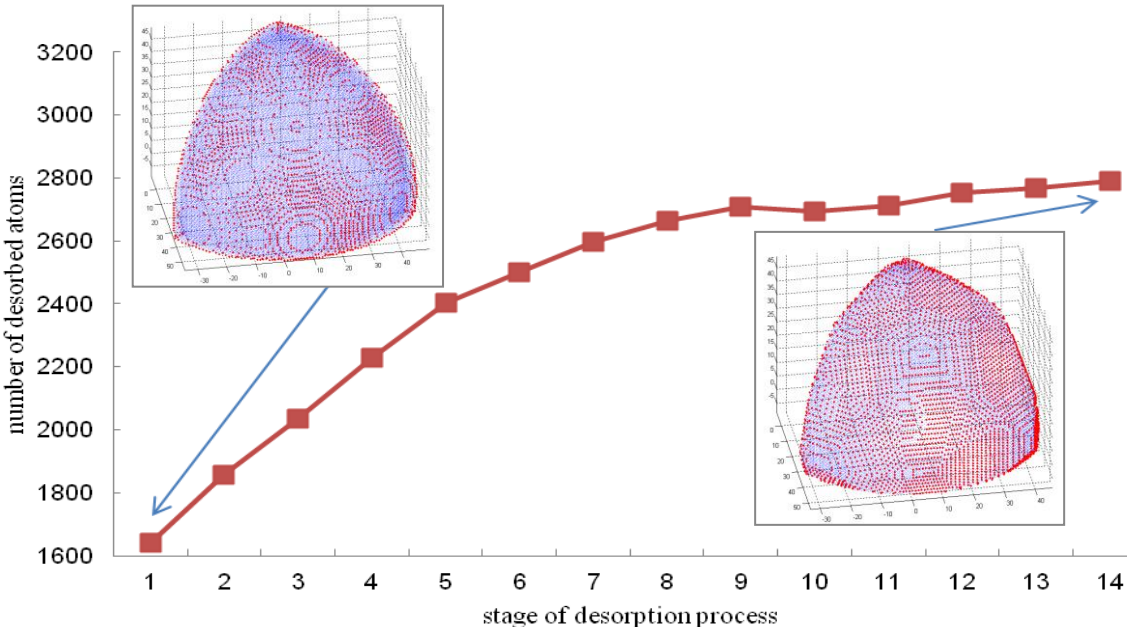


Figure 1. Number of evaporated atoms at several stages of field desorption process. Insets show surface configuration at the first and the last stages (surface atoms are shown in blue, desorbed atoms are marked red).

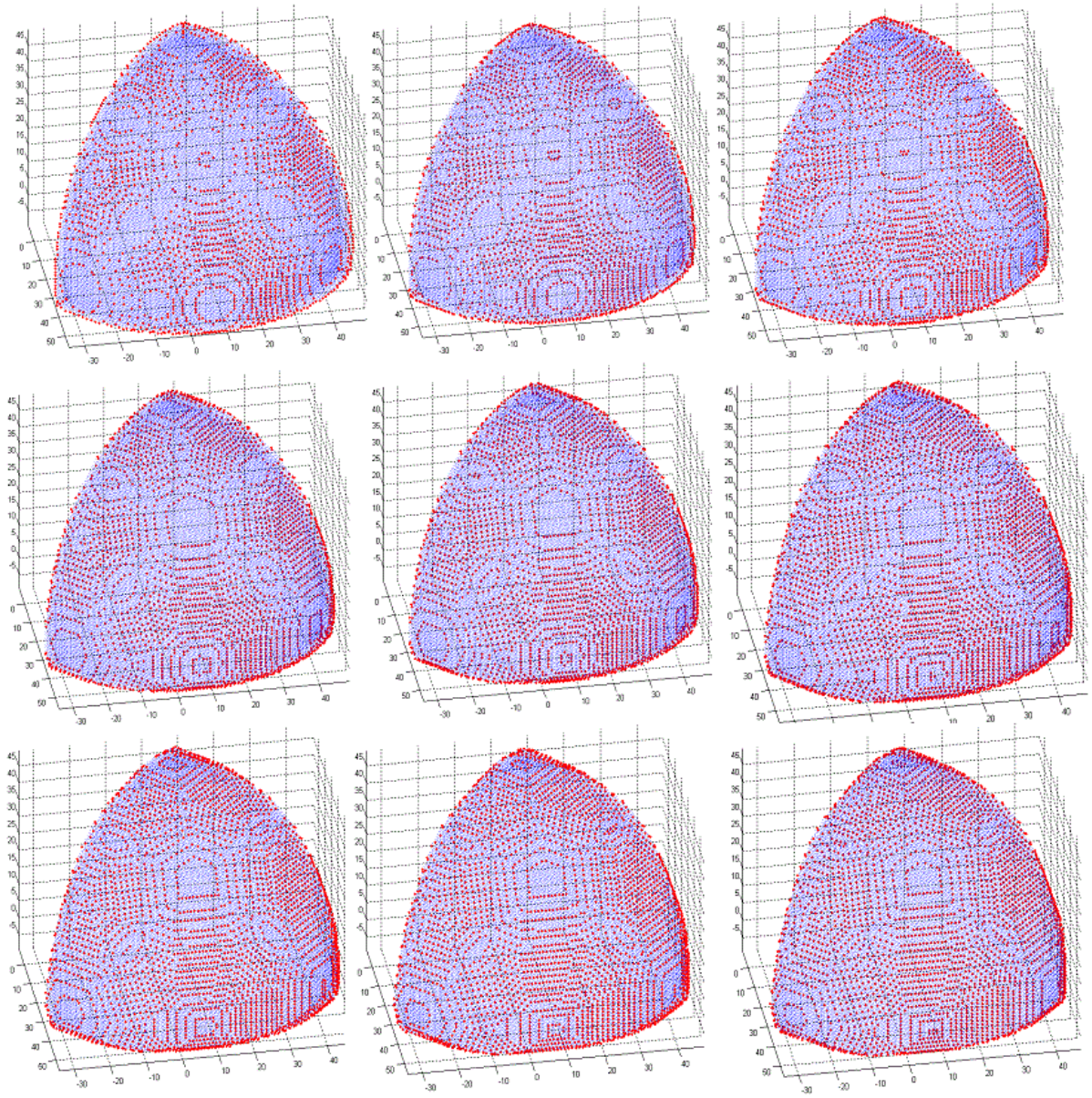


Figure 2. Several stages of field evaporation in the model of emitter tip surface segment.

4. Conclusion

In this paper we've constructed a model of emitter surface formed by the process of field-temperature evaporation. Some of the crystallographic faces of the emitter surface grew in this process relative to the initial shape (described in [2]). Thus, we can see how in field-temperature evaporation the structure of the emitter surface becomes more regular, which can have practical application for making experimental conditions for study of adsorption more precisely defined and predictable [3]. In this paper we have assumed the electric field constant, although it is known that field distribution is influenced by the surface structure that changes due to desorption. On the other hand, we do take into account those changes while calculating the binding energies. Even this simplified approach requires a considerable amount of computational resources, which makes studying of its computational complexity and looking for ways to increase its efficiency an important area of future research [16-18].

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