LOW TEMPERATURE CATHODE OPERATION: A SPOT MODEL-PART I

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Abstract

The problem of arc ignition from micropoints on an MPD cathode is considered, as a function of surface temperature, electric field and cathode material. A physical model of a micropoint has been developed and a relevant numerical code has been implemented. Model results for pure tungsten and thoriated tungsten cathodes are shown and discussed. The role of the Nottingham effect in the operation of the micropoints and in the explosive character of the cathode spot ignition is highlighted by the results. The model indicates the micropoint ignition is eased by a reduction of the material work function; the opposite happens with an increase of the base temperature. A larger number of activated micropoints means more spots that substain the discharge current and thus the overall erosion is reduced. These results are consistent with experimental evidences obtained with heated MPD cathodes, made of tungsten and thoriated tungsten.

List of symbols

A	Area of the generic micropoint cross section.
A_i	Area of the section i.
A_L	Area of the micropoint tip.
C_p	Specific heat capacity, [J/(kg K)].
e	Elementary charge.
F	Electric field.
h	Planck constant.
$\hbar$	$=h/4\pi$.
j	Current density at the generic micropoint section.
j_L	Current density at the micropoint tip.
k	Boltzmann constant.
m	Electronic mass.
p_z	Momentum along the z direction.
p_y	Momentum along the y direction.
T	Temperature.
T_0	Bulk cathode temperature.
T_i^n	Temperature of section i at the time t_n.
T_L^n	Temperature of the tip at the time t_n.
Δt	Time step.
W_a	Bottom level of the conduction band.
x_i	Coordinate of the section i.
x_L	Coordinate of the tip.
Δx	Space step.
ε_0	Permittivity of vacuum.
$\bar{\varepsilon}$	Average energy of the emitted electrons.
φ	Work function.
κ	Thermal conductivity, [W/(m K)].
ρ	Mass density.
σ	Electrical conductivity.
ζ	Fermi level.

Introduction

Cold cathode operation in MPD thrusters is characterized by a spotty current emission from the electrode surface. This emission regime involves intensive cathode erosion due to material evaporation and droplet ejection from the spots[1] leaving on the surface a number of crater-like pits. Tests carried out at Centrospazio have shown the cathode material and temperature not only determine the current emission regime (from spotty (cold) emission to diffuse (hot) emission), but also affect the spot operation itself, and consequently the surface damage on a relatively cold electrode[2]. On pure tungsten cathodes, crater dimension has been observed to increase with the base temperature, according to other experimental results and model predictions[1,3] while the opposite was observed on thoriated tungsten cathodes[4].

This different behavior has been only qualitatively explained so far: in a thoriated cathode, the heating yields a certain degree of surface coverage by thorium atoms, that lows the work function, making easier the ignition of a greater number of emission sites on the surface with respect to a heated electrode made of pure tungsten. The single spot has thus to sustain a minor current and, in turn, less energy is available for erosion processes.

To assess the experimental evidences in a more detailed and quantitative manner, a cathode spot model has been developed. This paper describes the

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first part of the model, dealing with the spot ignition. The second part, concerning the operation of a well-developed spot, will be discussed in another paper, to be presented in a next conference.

In the first part, the model considers the thermoelectric phenomena that make a surface micropoint of assigned geometry to develop in a emission site; in particular the model identifies the conditions in terms of base temperature, electric field and work function necessary for ignition. The pure tungsten and the thoriated tungsten cases have been considered and the relevant results are illustrated below.

Qualitative description

On the cathode surface, consider a micropoint whose tip is subjected to an elevated electric field. This is thought to be the situation immediately before the discharge in every vacuum or low gas pressure tube[5,6,7,8,9]. In correspondence of micropoints and other imperfections on cathode surface (i.e. lattice defects, inclusions etc.), the nominal electric field is amplified by a factor estimated in the order of 50 - 100.

Due to the electric field, electrons are able to escape from the potential barrier at the metal-vacuum boundary, generating an electron current through the micropoint. Since the characteristic values of the electron current density are very high, the micropoint undertakes a thermal runaway process that soon leads to the melting of the tip. This phenomenon has likely an explosive character and yields the release of a plasma cloud. This plasma provides the charged particles necessary for the vacuum breakdown between electrodes. From this moment, the micropoint has become a spot through which part of or the entire arc current passes as long as conditions are favorable in that point of cathode surface.

Electron emission overview

The electron current density emitted from the micropoint (and eventually from the spot) depends on the conditions of the emission site in terms of temperature and potential barrier that in turn depends on the external electric field[10].

The potential barrier, namely the energy potential field that prevents electrons from leaving the metal turns out to be:

$$V(x) = -W_a \qquad \text{for } x \le 0$$

$$V(x) = -\frac{e^2}{4\cdot\pi\cdot\varepsilon_o\cdot(4\cdot x)} - e\cdot F\cdot x \qquad \text{for } x > 0$$

x is the space coordinate perpendicular to the surface and pointing out of the metal body.

The reference level for the potential energy belongs to the situation of the electron at an infinite distance from the surface.

Except for the cases of thermionic and field emission for which specific equations have been found[10,11], electron current density can be calculated as:

$$j(T,F,\zeta) = e\int_{-W_a}^{\infty} N(T,\zeta,W)D(F,W)\,dW \qquad (1)$$

$N(T,\zeta,W)$ is called supply function and NdW represents the number of electrons with energy in the interval W, $W+dW$ impinging over the potential barrier. W is the sum of the potential energy and the kinetic energy due to the motion in the x direction.

$N(T,\zeta,W)$ derived from the Fermi-Dirac statistics has the following form:

$$N(T,\zeta,W) = 4\,m\,kT\,h^{-3}\ln\{1+\exp[-(W-\zeta)/kT]\}$$

Due to the chosen reference level for energies, note that $-\zeta$ is simply the value of the material work function.

$D(F,W)$ is called transmission coefficient and represents the probability that an electron with energy W tunnels the potential barrier:

$$D(F,W) = \left[1+\exp\left(-2i\hbar^{-1}\int_{x_1}^{x_2}\sqrt{2m(W-V(x))}\,dx\right)\right]^{-1}$$

x_1 and x_2 are the zeroes of the integrand.

In the following, in order to calculate the electron current density emitted from the micropoint, the approximation for $D(F,W)$ reported in ref.[10] has been used.

The integral in (1) is extended all over the possible values of the total energy.

An interesting thermal effect is associated to electron emission, named Nottingham effect[12]. The emitted electrons are replaced inside the lattice by the conduction electrons having an average energy equal to the Fermi level. Depending on the average energy of the emitted electrons, the emission can thus cool or heat the metal.

The average energy of the emitted electrons is given by:

$$\bar{\varepsilon} = \frac{\int_{-W_a}^{\infty} D(W) \left\{ \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{\left(W + \frac{p_y^2 + p_z^2}{2m}\right) dp_y dp_z}{1 + \exp\left(\frac{W-\zeta}{k\cdot T} + \frac{p_y^2 + p_z^2}{2mkT}\right)} \right\} dW}{\int_{-W_a}^{\infty} D(W) \left\{ \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{dp_y dp_z}{1 + \exp\left(\frac{W-\zeta}{k\cdot T} + \frac{p_y^2 + p_z^2}{2mkT}\right)} \right\} dW}$$

For a given electric field, a critical temperature value, T^*, exists: for temperature larger than T^* , $\bar{\varepsilon} > -\zeta$ and the emission site is cooled, while the viceversa happens for T smaller than T^*.
T^* is given by[13]:

$$T^* = \frac{ehF}{8\pi k (2m\phi)^{0.5}}$$

Nottingham effect extends as far as a few interatomic distances under the surface.

The model

The micropoint is sketched as a truncated cone; if the area of the cross section varies slowly, temperature and current density can be considered uniform on every section and they only depend on the x coordinate along the micropoint axis.
In this situation the thermal conduction equation is[13]:

$$\rho C_p \frac{\partial T}{\partial t} A dx = -\left(\frac{\partial (qA)}{\partial x} dx\right) + (jA)^2 \frac{1}{\sigma} \frac{dx}{A} \qquad (2)$$

where:

$$q = -\kappa \frac{\partial T}{\partial x} - \frac{j}{e}\zeta \qquad (3)$$

If the electron current is emitted only from the tip of the micropoint, the total current crossing each section is constant and the second term in the expression of q does not contribute in the equation (1).
Boundary conditions are:

$$T|_{x=0} = T_0$$

$$\kappa \frac{\partial T}{\partial x}\bigg|_L = -\frac{j(T,F,\zeta)}{e}\left(\bar{\varepsilon}(T,F,\zeta) - \zeta\right) \qquad (4)$$

Note that the second term in (3) is very important in writing the boundary condition (4): it accounts for the the average energy of electrons replacing those emitted from the tip.
The initial condition is obviously:

$$T=T_0$$

Because the temperature range is very large (from 300 K to the material melting point (3680 K for tungsten)), material properties are considered temperature dependent.
For the specific heat capacity and the thermal conductivity, the following expressions are obtained from experimental data interpolation[14]:

$$C_p(T) = 22.76 \cdot \left(5.59 + 7.30\cdot 10^{-4} T + 1.51 \cdot 10^{-7} T^2\right)$$

$$\kappa(T) = 112.44 - 1.13\cdot 10^{-2} T + \frac{20221.63}{T}$$

For the electrical conductivity, the Wiedemann-Franz law is used[13]:

$$\frac{\kappa}{\sigma \cdot T} = \frac{1}{3}\left(\frac{\pi k}{e}\right)^2$$

Substituting this last expression in (2), the conduction equation assumes the final form:

$$\rho C_p \frac{\partial T}{\partial t} = \kappa \frac{\partial T}{\partial x}\frac{1}{A}\frac{dA}{dx} + \frac{\partial \kappa}{\partial x}\frac{\partial T}{\partial x} + \kappa \frac{\partial^2 T}{\partial x^2} + j^2 \frac{T}{3\kappa}\left(\frac{\pi k}{e}\right)^2 \qquad (5)$$

It holds until the tip temperature reaches the melting point. According to some literature, this event coincides with cathode spot ignition. A new physical model is necessary for describing heat and current transport in the spot.

Solution

Micropoint dimensions are fixed as reported in Fig. 1. They likely are those of some irregularities on a machined surface.
Chosen a series of points along the micropoint axis, equation (5) is transformed in a finite difference equation for each point, assuming that the temperature does not vary in the volume of height Δx around the point.
In particular the Crank-Nicholson method is used: being an implicit method, it presents the advantage of a greater stability respect to an explicit one.
For the generic point x_i the finite difference equation is:

$$\rho C_p \frac{T_i^{n+1} - T_i^n}{\Delta t} = \left(\frac{\kappa(x_i)}{A_i} \frac{dA}{dx} + \frac{\kappa\left(x_i + \frac{\Delta x}{2}\right) - \kappa\left(x_i - \frac{\Delta x}{2}\right)}{\Delta x} \right) \cdot \left[\frac{\frac{1}{2}\left(T_{i+1}^{n+1} + T_{i+1}^n\right) - \frac{1}{2}\left(T_i^{n+1} + T_i^n\right)}{\Delta x} \right] +$$

$$+ \kappa \left[\frac{\frac{1}{2}\left(T_{i+1}^{n+1} + T_{i+1}^n\right) + \frac{1}{2}\left(-2 \cdot T_i^{n+1} - 2 \cdot T_i^n\right) + \frac{1}{2}\left(T_{i-1}^{n+1} + T_{i-1}^n\right)}{\Delta x^2} \right] + \left(\frac{A_L \, j_L\left(T_L^n, F, \zeta\right)}{A_i} \right)^2 \left(\frac{T_i^{n+1} + T_i^n}{2} \right) \frac{1}{3\kappa(x_i)} \left(\frac{\pi k}{e} \right)^2$$

As can be noted, material properties are evaluated at the time t_n; this allows the system keep linear in the T_i^n variables.

The hypothesis of uniform temperature in the finite volume around x_i is not true near the tip of the micropoint, where temperature gradients are very high, primarily for the Nottingham effect. This not only imposes a tighter mesh in that zone, but makes the finite difference equation to be written in a different way. In fact for the volumes near the tip the conduction term is expressed as difference from output and input heats:

$$\rho C_p \frac{T_i^{n+1} - T_i^n}{\Delta t} A_i \Delta x = \kappa\left(x_i - \frac{\Delta x}{2}\right) \frac{\frac{1}{2}\left(T_{i-1}^{n+1} + T_{i-1}^n\right) - \frac{1}{2}\left(T_i^{n+1} + T_i^n\right)}{\Delta x} A\left(x_i - \frac{\Delta x}{2}\right) +$$

$$+ \kappa\left(x_i + \frac{\Delta x}{2}\right) \frac{\frac{1}{2}\left(T_{i+1}^{n+1} + T_{i+1}^n\right) - \frac{1}{2}\left(T_i^{n+1} + T_i^n\right)}{\Delta x} A\left(x_i + \frac{\Delta x}{2}\right) + \left(\frac{A_L \, j_L\left(T_L^n, F, \zeta\right)}{A_i} \right)^2 \left(\frac{T_i^{n+1} + T_i^n}{2} \right) \frac{1}{3\kappa(x_i)} \left(\frac{\pi k}{e} \right)^2$$

The boundary condition (4) becomes:

$$\rho C_p \frac{T_L^{n+1} - T_L^n}{\Delta t} A_L \frac{\Delta x}{2} = \kappa\left(x_L - \frac{\Delta x}{2}\right) \frac{\frac{1}{2}\left(T_{L-1}^{n+1} + T_{L-1}^n\right) - \frac{1}{2}\left(T_L^{n+1} + T_L^n\right)}{\Delta x} A_L +$$

$$- \frac{j_L\left(T_L^n, F, \zeta\right)}{e} \left(\bar{\varepsilon}\left(T_L^n, F, \zeta\right) - \zeta \right) + \left(j_L\left(T_L^n, F, \zeta\right) \right)^2 A_L \frac{\Delta x}{2} \left(\frac{T_L^{n+1} + T_L^n}{2} \right) \frac{1}{3\kappa(x_L)} \left(\frac{\pi k}{e} \right)^2$$

About the choice of the appropriate space and time steps adopted in the solution, the following considerations have been done.

Since equation (5) holds for a continuum medium, the minimum space step is taken equal to 100 times the interatomic distance. As shown in Fig. 2, the mesh consists of three zones. The first, close to the micropoint base, has the larger step size *dx*; the tip zone presents a tighter mesh with the smallest step size *dx'*; finally, in the intermediate zone, step size changes exponentially from *dx* to *dx'*.

The time step is chosen such that thermal equilibrium can be reached inside the single volume. Thermal processes involved are characterized by the time between two subsequent collisions of an electron against the lattice.

This time has been evaluated for tungsten at different temperatures by means of the following relation[15]:

$$\tau = \frac{m\sigma}{n e^2}$$

where n is the number of free electron per unit volume and has been safely assumed equal to 6.3 $10^{28}/m^3$, which means there is one free electron per tungsten atom. Assuming that equilibrium is reached after about 100 collisions per electron, the minimum time step has been calculated to be 10^{-12}.

The linear system obtained after writing all equations is solved with the Gauss method. Current density from the tip and the average energy of emitted electrons are calculated applying the Simpson method to solve the integrals in the expression of $D(F,W)$ and $\bar{\varepsilon}$.

The electric field at the micropoint tip is found by attempts, provided the micropoint reach the melting point in a time ≤ 1 ns. This limit has been established, considering that many experimental observations

reveal spot activity on the cathode surface after some nanoseconds.
The stability of the numerical solutions has been verified, reducing the time step without appreciable difference in the numerical results.

Results and discussion

The aim of this investigation is to highlight the role of temperature and surface work function on cathode spot operation in an MPD thruster. Thus the solution of the model has been carried out for particular values of the parameters entering in the equations.
Tungsten has been considered as cathode material.
Temperature of the electrode bulk (T_0) has been varied between 300 and 2000 K.
Regarding the work function values adopted, previous researches showed the importance of thorium surface coverage on the current emission regime[2,4]. Therefore, the work function has been varied from the value of 4.5 eV belonging to a pure tungsten surface to the value of 2.7 eV, the minimum value that can be obtained from thorium coverage on tungsten. Note that these work function values are consistent with the chosen temperatures[16].
Tab. 1 shows the value of the electric field that leads the micropoint tip to melting for different cathode bulk temperatures and for a work function value of 4.5 eV. The last column of the same table reports the values of the current density at the tip just before melting.
The relevant data for a work function value of 2.7 eV are presented in Tab. 2.
The order of magnitude of electric field and current density agree with results from other investigations[7,8,9].
The electric field necessary for cathode spot ignition weakly decreases with T_0, while a stronger dependence on work function results. Going from 4.5 eV to 2.7 eV the electric field decreases by a factor of 0.5.
The same trend is shown by data referring to the condition of micropoint melting in 0.1 ns.
On the surface of an electric thruster cathode the electric field undertaken by each micropoint is equal to the nominal electric field intensified by a factor that depends on the specific micropoint geometry. If the critical value of the electric field leading to micropoint melting decreases, probably more micropoints have at their tip an electric field greater than this value and thus more spots are contemporary activated on the surface. This means the total arc current is emitted in a more diffuse way, likely involving a less surface damage.
Model results indicate that the main benefit derives from the work function decrease rather than from the cathode temperature increase. However, work function decrease is due to thorium surface coverage, obtained by cathode heating.
Recent experiments at Centrospazio agree with these theoretical results[2]. In fact thruster operation with a pure tungsten cathode has shown that electrode heating induces a more intense surface damage: craters left by spots are greater than those remaining on the surface after cold operation. In fact, in a pure tungsten cathode any beneficial effect by thorium is precluded and the same number of spots sustains the arc current, independently from cathode temperature. According to several spot models[1,3,17], erosion induced by spot operation on a relatively hot surface is stronger than on a cold surface.
On the other hand, past experiments on 2% thoriated tungsten cathode[18] have shown an opposite trend which can now be justified: due to surface thorium coverage, on the hot cathode more spots were ignited than on the cold electrode. Sustaining a minor current, the spot on the heated surface induces less erosion than on a cold surface.
Other observations can be made from the numerical solution of the micropoint model:

- temperature in the micropoint is almost uniform along the x coordinate, except for the tip region where it steeply increases. The characteristic profile is shown in Fig. 3, while Fig. 4 is a zoom of the temperature profile in the tip region.
- For each point, temperature increases monotonically with time, but the increment reduces progressively.
- At the beginning, Nottingham effect prevails on the other thermal effect. As long as the tip temperature is smaller than the inversion temperature, Nottingham effect brings heat to the volumes in the tip region. When the inversion temperature is overcome, Nottingham effect cools the tip region; anyway at this point heating mechanisms are dominant and the temperature continues to raise. In fact due to the increase of the emitted current and of the electrical resistivity with temperature, Joule heating is very strong; moreover cooling by conduction is not efficient at high temperatures because of conductivity reduction.
- Due to the cooling induced by the Nottingham effect at the end of the process, melting temperature is reached in a point under the tip (the model can not distinguish the two points). This last circumstance seems explain the explosive character of cathode spot ignition as observed many times. The explosion is likely caused by pressure exerted by the melt on the solid tip.

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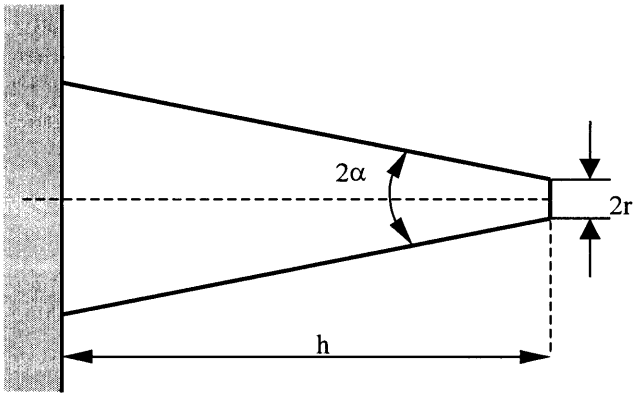


Fig. 1 Micropoint geometry: h=10μm, r=.2μm, α=30°.

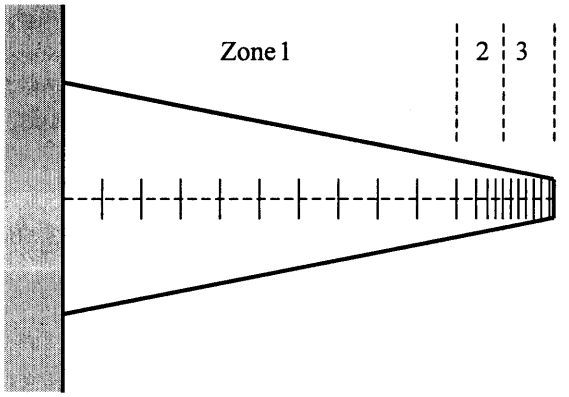


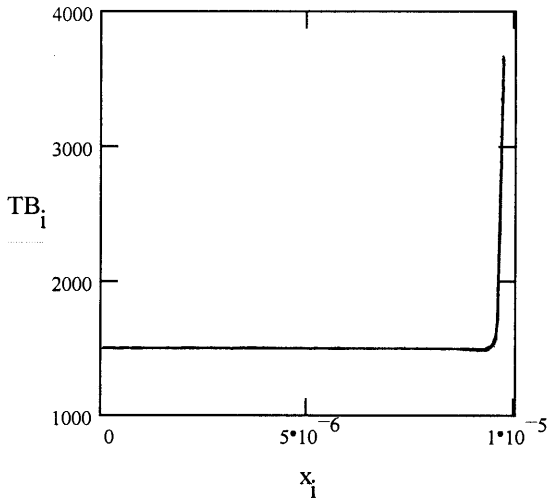
Fig. 2 Mesh along the *x* coordinate (steps are only representative).

Bulk temperature $T_o(K)$	Electric field $F(V/m)$	Current density $j_L\ (A/cm^2)$
2000	$1.089 \cdot 10^{10}$	$1.626 \cdot 10^{9}$
1500	$1.103 \cdot 10^{10}$	$1.734 \cdot 10^{9}$
300	$1.136 \cdot 10^{10}$	$2.006 \cdot 10^{9}$

Tab. 1 Electric field and current density at the micropoint tip just before melting for φ=4.5 eV.

Bulk temperature $T_o(K)$	Electric field F(V/m)	Current density $j_L(A/cm^2)$
2000	$5.20 \cdot 10^{9}$	$2.416 \cdot 10^{9}$
1500	$5.275 \cdot 10^{9}$	$2.537 \cdot 10^{9}$
300	$5.475 \cdot 10^{9}$	$2.875 \cdot 10^{9}$

Tab. 2 Electric field and current density at the micropoint tip just before melting for φ=2.7 eV.



TB =

	0
27	1502.14
28	1503.31
29	1505.73
30	1511.04
31	1522.68
32	1547.5
33	1598.57
34	1700.7
35	1904.68
36	2342.49
37	3685.27

Fig. 3 Characteristic profile of temperature along micropoint axes (TB in K and x_i in m).

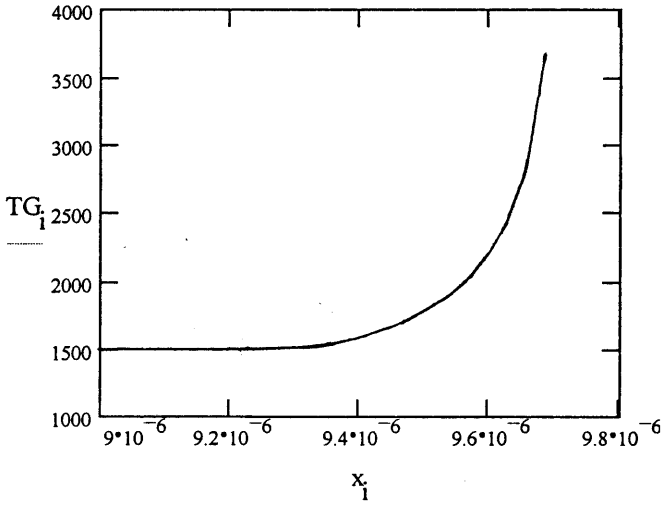


Fig. 4 Temperature in the micropoint tip region (TG_i in K and x_i in m).