The physics of ion impact cathode heating

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The heating of a metal surface by ion impact is described by a coupled electron and phonon model that follows from recent research on femtosecond laser heating of metals. The conduction electrons of the metal are directly heated to very high temperature by the impinging ion and then on a longer time scale transfer their energy to the lattice. This results in very efficient heating of the lattice. These processes are described by coupled partial differential equations for the electron and lattice temperatures. The results from three-dimensional numerical solutions of these equations are presented.

I. INTRODUCTION

Evidence now exists that the prevalent concept of how ions heat the cathode of a discharge may be incorrect. We will propose a different approach to the problem based on recent research into the heating of metals by short pulse lasers.

For many years the gas discharge community has assumed that the cathode in a high current discharge is heated by collisions of energetic ions with the lattice of the metallic surface. Typical of the arguments presented is that stated by Cobine in his classic treatise on gas discharges.[1] Summarizing arguments presented by Thomson and Loeb explaining thermionic emission in electric arcs, Cobine notes that the ion current densities and ion kinetic energies, which are gained as the ions traverse the potential drop in the cathode sheath, are high enough to heat the top 10^{-5} cm of a copper cathode to 4000 °C in less than 10^{-4} s.

The issue of how hot a cathode may become has arisen recently in the experiments of Hartmann and Gundersen[2,3] on short pulse, high current hollow cathode discharges (also known as pseudosparks) in H_2 (see also the recent modeling performed by Sommerer *et al.*[4]). Such devices may operate with current densities of 10^4 kA/cm^2 or greater and cathode potential drops of 100 V or more. Power densities impinging on the cathode may be 10–20 MW/cm^2. Hartmann and Gundersen performed estimates of the temperature of the cathode due to ion impact heating using known analytical solutions to the heat equation.[5] The temperature change near the surface of a semi-infinite metal slab being heated by a time dependent flux of power, $F(t)$, at the surface can be computed using the relation

$$\Delta T(z,t)=\frac{\kappa^{1/2}}{K\pi^{1/2}}\int_0^t F(t-\tau)\exp\left(\frac{-x^2}{4\kappa\tau}\right)\frac{d\tau}{\tau}, \qquad (1)$$

where K is the thermal conductivity, $\kappa=K/(\rho c)$ is the thermal diffusivity, c being the specific heat and ρ the mass density. Equation (1) arises from the Green function,

$$\Delta T(r,t)=\frac{Q}{8(\pi\kappa t)^{3/2}}e^{-r^2/4\kappa t}, \qquad (2)$$

where Q has units of K/cm^3 and $Q\rho c$ is the energy deposited by an instantaneous point source at $t=0$ and $r=0$. The temperature change at the surface of the slab for a constant flux F_0 is given by

$$\Delta T(0,t)=\frac{2F_0}{K}\left(\frac{\kappa t}{\pi}\right)^{1/2}. \qquad (3)$$

Using Eqs. (1) and (3) Hartmann and Gundersen found that power densities in the range 10–20 MW/cm^2 for times less than or equal to about 100 ns were required to heat a thin surface layer to the approximately 2900 K melting point of molybdenum, which was the cathode material. They had found evidence of surface melting of the cathode in their experiments. This power flux corresponds to current densities of 5×10^4 to 10^5 A/cm^2 of 200 eV protons bombarding the surface. Hartmann and Gundersen[2,3] find an inconsistency between the estimated current density required to heat a cathode to high enough temperature for significant thermionic emission and the estimates of what the ion current densities actually are in the experimental devices. Because the thermal conductivity actually decreases[6] by about $\frac{1}{3}$ between 300 and 2800 K and then drops by another 20% at the melting point, the estimated temperatures should probably be somewhat higher. This, however, does not explain the inconsistency.

II. HEATING OF ELECTRONS AND COUPLING TO LATTICE

A. Theory

Drawing on recent advances in understanding the physics of heating of metal surfaces by femtosecond lasers, we are proposing herein a new picture of how metals are heated by ion impact. This picture leads us to believe that, in the cathode heating problem discussed above, the metallic surface of the cathode may be heated by quite high temperatures by a significantly smaller ion current density than previously thought.

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Over the past decade increasingly sophisticated experiments using femtosecond lasers have been performed on the heating of the electrons in a metal and the subsequent energy transfer to the lattice.[7–13] It has been found that the Fermi degenerate electrons in the metal target are heated to quite high temperatures due to their small heat capacity. This energy is then coupled to the lattice on a half picosecond or longer time scale. If we examine the physics of low energy proton collisions with a metal surface, such as Mo or W, we find that, because the nuclear stopping power is much smaller than the electronic stopping power,[14] most energy is deposited in the electrons between collisions of the proton with the ionic cores. Although a proton will transfer more energy to an ionic core in a headon collision, the energy transfer from the proton to the electron gas via long range Coulombic collisions is much more efficient than transfer to the ionic cores via a screened Coulombic interaction. Thus as a proton slows down in a metal it transfers much of its energy to the electrons. In addition, it will be neutralized by electron capture at some point in its trajectory and may even go through a series of neutralization-reionization events. Lakits *et al.*[15] have provided some theory on this process for slow protons in metals, including the ratio of the stopping power for H atoms to that of protons in a metal. For a typical range of metallic densities they find that the stopping power for neutral H is about 50%–70% of that for protons. Thus, even with neutralization most energy is still transferred to the electrons.

Given that the electrons are preferentially heated when an ion collides with a metal surface, the physics of ion impact heating of a metal lattice is very similar to that of heating using a femtosecond laser.[16] The proton energy is deposited in the electron gas along a track of some depth into the surface and the energy is eventually transferred to the lattice from electrons. Simulations performed using the TRIM[17,18] Monte Carlo code show the average proton penetration depths to range from 10 Å at 20 eV to 70 Å at 500 eV with average path lengths ranging from 27 to 304 Å, respectively.

We have investigated the heating of a metal surface by ion impact by numerically solving the coupled electron and lattice heat equations in three dimensions. The equations for the electron temperature T_e and the lattice temperature T_l are[19]

$$c_l \frac{\partial T_l}{\partial t} = K_l \nabla^2 T_l - g(T_l - T_e) + \frac{\partial K_l}{\partial T_l} (\nabla T_l)^2 + Q_l(t), \tag{4a}$$

$$c_e \frac{\partial T_e}{\partial t} = K_e \nabla^2 T_e + g(T_l - T_e) + \frac{\partial K_e}{\partial T_e} (\nabla T_e)^2 + Q_e(t). \tag{4b}$$

In general the electron and lattice specific heats, c_e and c_l, and the thermal conductivities, K_e and K_l, are temperature dependent. c_l is approximately constant and equal to $3Nk$ for lattice temperatures greater than the Debye temperature (T_D=450 K for Mo). c_e increases linearly in the Fermi degenerate region from zero at $T_e=0$, begins flattening out at $T_e=T_F/10$, and approaches $3n_ek/2$ for

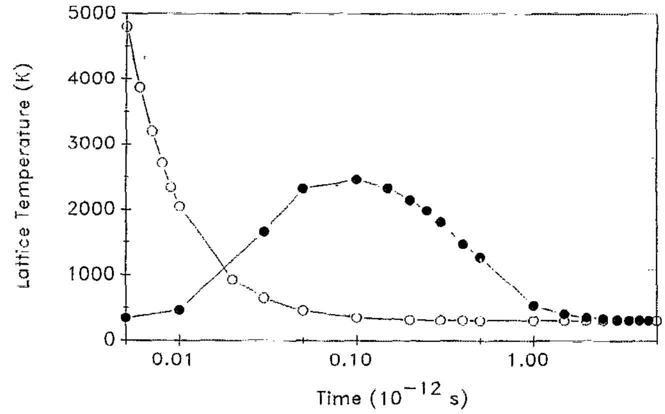

FIG. 1. Lattice temperature as a function of time for finite slab: (○) single temperature model and (●) coupled electron-phonon model.

$T_e \simeq T_F$ ($T_F=8.5\times10^4$ K for Mo). The lattice thermal conductivity is approximately inversely proportional to the lattice temperature and has a value that is a tenth or less of the electron thermal conductivity. In the calculations to follow we have taken $K_l=0.1K_e$ at 300 K. The electron thermal conductivity is a function of both the lattice temperature and the electron temperature. Following the work of Corkum *et al.*[10] we have used Sommerfeld's model[20] to compute the electron thermal conductivity. Thus $K_e=v_F^2\tau c \propto T_e/(\nu_e+\nu_l)$, where ν_e and ν_l are respectively the electron-electron and electron-phonon collision frequencies. The total collision frequency $\nu_e+\nu_l=\nu_0 \times[(1-\beta)T_l/300+\beta(T_e/300)^2]$ where $\beta=\nu_e/\nu_l\simeq0.5$ for transition metals.[21] ν_0 is then obtained from the thermal conductivity at 300 K. In our calculations we used a flux-limited formulation[22] for the heat flux that is commonly used in laser–plasma interaction modeling. The electron heat flux is given by $q_e^{-1}=q_d^{-1}+q_{fs}^{-1}$, where q_d is the diffusive flux and q_{fs} is the free streaming flux.

The electron-lattice coupling coefficient, g, is given for the situation where $T_l,T_e \gg T_D$ by[16]

$$g=\frac{\pi^2}{6}\frac{mn_ev_s^2}{\tau_{ep}T_l}, \tag{5}$$

where m is the electron mass, n_e the electron density, v_s the sound velocity, and τ_{ep} is the electron-phonon collision time. Because τ_{ep} is inversely proportional to the lattice temperature T_l, g is a constant independent of T_l. We have taken $g=5\times10^{11}$ W/cm^3 K, which is in the range estimated for tungsten by Fujimoto *et al.*[7] from their laser experiments.

B. Calculations

Figure 1 shows the time dependence of the temperature in the center of the surface of a slab due to a single proton impact. This is from a three-dimensional calculation using a one temperature model with specific heat c=0.25 J/g/K and thermal conductivity K=1.38 W/cm/K, which are the values for bulk Mo. This result is in agreement with the result obtained using the analytical

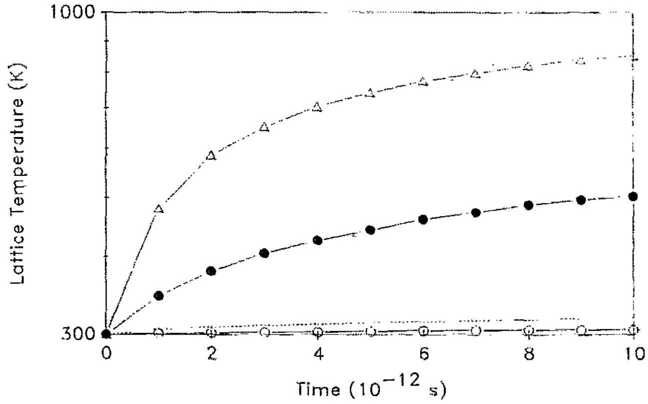

FIG. 2. Lattice temperature as a function of time for simulated semi-infinite slab: (----) theory using Eq. (3) and bulk Mo heat capacity and thermal conductivity for $F_0=10$ MW/cm^2; the curves with symbols are calculations using the coupled electron-phonon model for different values of power flux, F_0; (△) 10 MW/cm^2, (●) 5 MW/cm^2, and (○) 2.5 MW/cm^2.

Green function.[23] In this calculation a 500 eV proton has deposited all its energy in the top 20 Å of a 200 Å×200 Å×300 Å Mo slab. The sides and bottom of the slab were held at 300 K. Figure 1 also shows a calculation performed for the same problem using the coupled electron and lattice model of Eqs. (4), whereby the electrons are heated by the impinging ion and then slowly transfer their energy to the lattice. We have neglected the possibility of "knock-on" electrons that would travel ballistically away from the track of the proton. This and our assumption that all proton energy is transferred to the electrons in a distribution that remains thermal probably somewhat overestimates the initial electron heating. We see that the time scale for achieving the same temperatures in the tail of the heat pulse is an order of magnitude longer than in the one temperature calculation. Consequently, for a sequence of proton impacts over a period of time, one would expect that the temperature will be greater than predicted using the conventional method. In terms of current density, a smaller current density is required to heat a cathode to a given temperature than one would predict using Eq. (1).

To examine what happens when a continuous flux of ions is bombarding a surface we performed Monte Carlo calculations solving Eqs. (4) using a source term Poisson distributed in time with a collision frequency proportional to the current density. We approximated a semi-infinite slab, appropriate for the short time scales under investigation, by using periodic boundary conditions on the sides of the slab in the x and y dimensions. We changed the incident power flux by retaining a constant current density of 5×10^4 A/cm^2 and varying the proton impact energy. Figure 2 shows the results of these simulations for F_0=2.5, 5, and 10 MW/cm^2 along with the 10 MW/cm^2 theoretical curve from Eq. (3) for ΔT at the surface of slab. We see that, as expected, the slab gets significantly hotter at a power flux of 10 MW/cm^2 than predicted using the formula of Eq. (3). All heating curves have approximately a $t^{1/2}$ time dependence. On the long time scales typical of ordinary arc discharges, when the system is in a steady state, the differences between this picture of the heating mechanism and that involving direct heating of the lattice will be negligible. The functional dependence on flux does not appear simple. The relationships between ion energy, ion mass, current density, and material properties and the heating rate will require intensive further investigation. Additionally, we have picked a value for the lattice thermal conductivity for the sake of our point but have not thoroughly investigated how the results depend on the value of K_l. Finally, although the electrons are heated transiently to quite high temperature, their direct contribution to thermionic emission is quite small due to the short time scales and small spatial dimensions over which the heating occurs. Even if the entire 200 Å×200 Å surface were heated to 10 eV by the proton impact and T_e had a 1 ps decay time, the probability of an electron being emitted would be only 0.07, less than the coefficient for potential emission.

III. FURTHER ISSUES AND CONCLUSIONS

Although more complicated than the one temperature model of heating, this model is itself rather simplified in that there are several other effects that may add complexity. There is the possibility of surface melting, which can occur at temperatures below the bulk melting temperature.[24,25] On short time scales the issue of melting versus superheating[26,27] is complex and not yet well understood. Melting will enhance heating to some extent due to the lower thermal conductivity of the liquid metal. At some point, however, the energy loss to radiation, particle emission, and sputtering will enter the temperature equations (4). There is evidence also that the sputtering threshold is lower and the sputtering yield greater for a liquid metal.[28]

The modeling is further complicated by the implications of recent femtosecond laser studies that show that the electrons themselves take as long as a picosecond to relax to a Fermi–Dirac distribution. It has always been assumed that the electron velocity or energy distribution relaxes to the Fermi–Dirac distribution on a time scale approximately equal to the electron–electron collision time, about 10 fs. Recent measurements,[13,29,30] however, indicate that the relaxation time scale may be more like a picosecond. These results may make the temperature equations (4) suspect and require more of a kinetic theory approach to the heating and electron–phonon coupling problem, such as solving Boltzmann's equation or performing Monte Carlo simulations. Some of these issues are discussed by Fann *et al.*[13,30]

In conclusion, we have examined the physics of ion impact heating of electrons in a metal surface and subsequent energy transfer to the lattice as a mechanism for cathode heating in a short pulse high current discharge. We find this two step process to be much more efficient at heating the metal surface than direct collisional heating of the lattice by the impinging energetic ions. This approach to modeling the cathode heating process helps to resolve the issue of anomalous electron emission in recent hollow cathode discharge experiments.[2,3] For instance, more recent analysis by Anders *et al.*[31] indicates that the maximum power density available to heat the surface is 3 MW/cm^2, which from Eq. (3) would take about 200 ns to heat the Mo cathode surface to its melting point. Our modeling indicates the heating time should be approximately 20 ns.

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