TEMPERATURE PROFILE AND DEPTH OF SURFACE MELTING OF A METAL IRRADIATED BY A HIGH-CURRENT ION BEAM


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We have numerically solved the nonlinear thermal conductivity equation using temperature-dependent thermal coefficients to study the evolution of the temperature profile produced in a metal irradiated by a high-current ion beam. We studied the propagation of the thermal front and the heating rate of the metal surface as functions of ion beam characteristics. We determined the dependence of the maximum heating temperature and penetration depth on the maximum value of the ion beam current.

Introduction

The temperature-phase modification of metal and alloy surfaces irradiated by high-power ion beam pulses is the subject of active research [1-3]. The analysis of high-current ionic treatment of metals is very valuable in reactor construction for predicting the durability of walls in thermonuclear reactors. Ion pulses are very effective for producing new construction materials with qualitatively improved physical, chemical, and mechanical surface properties. This research is also valuable in the rapidly-evolving microelectronics industry because of the possibility for producing drop-like nanostructures (clusters) of conducting materials, and of producing on semiconductor surfaces high densities of current carriers (quantum dots) that may aid in the further miniaturization of computer technology.

While ion-beam treatment of metals is about 10 years old, previously it was premature to consider the complete study of all physical processes involved in altering surfaces irradiated by high-current, pulsed, high-energy ions (at least to the same degree as experienced after irradiation by laser or electron beams). Because of the work of many researchers we can now understand the macroscopic details of surface heating during ion irradiation. That is, we can determine the temperature profile in the sample and the melting depth of the irradiated surface as a function of ion beam density for a high-current, short-pulse beam.

A primary factor determining sample heating during ion beam irradiation is the energy loss of the ions in the sample. Although the reliability of data concerning ion energy loss for a given energy range is not good [3], the experimental distribution of absorbed energy is well approximated by a piecewise linear dependence on the ion penetration depth: The absorbed energy first increases with depth, reaches a maximum, and then declines more slowly (see [3], Fig. 3.1).

In this paper we study the temperature profile and the melting depth as a function of the ion beam shape, taking into account the fact that the thermal properties of the material are temperature dependent. We also use boundary conditions that allow for the finite thickness of the sample, and the cooling effects of radiative heat exchange between the sample surface and the vacuum. Our goal in this study is to verify the use of the model for subsequent application to predicting thermoelastic processes. A further goal of the modeling process is to reveal which outputs of the model are sensitive to the choices of source function and boundary conditions.

1. The Model

To find the temperature field $T$ and its evolution, we have numerically solved the one-dimensional thermal conduction equation
\[
\rho c(T) \frac{dT}{dt} = \frac{\partial}{\partial x} \left( a(T) \frac{\partial T}{\partial x} \right) + Q(x, t),
\]

where \( \rho \) is the density of the irradiate sample, \( c(T) \) is the heat capacity, and \( a(T) \) is the thermal conductivity. The heat source \( Q(x, t) \) takes the form suggested in [3]:

\[
Q(x, t) = \begin{cases} 
\frac{E_0 j(t)}{zeR}, & t \leq \tau, \ x \leq R, \\
0, & t > \tau, \ x > R,
\end{cases}
\]

where \( \tau \) is the time the source is active, and \( E_0, j(t), ze, \) and \( R \) are the initial energy, current density, charge, and average ion mean free path, respectively. The ion beam current density \( j(t) \) used in our calculations is

\[
j_1(t) = \text{const} = \frac{j_{\text{max}}}{2},
\]

\[
j_i(t) = \begin{cases} 
\frac{j_{\text{max}} t}{\tau_i}, & t \leq \tau_i, \\
\frac{j_{\text{max}} (\tau - t)}{\tau - \tau_i}, & \tau_i < t \leq \tau,
\end{cases}
\]

where

\[
\tau_{2,3,4} = \frac{\tau}{2}, \frac{3\tau}{2}, \frac{3\tau}{4}
\]

and \( j_{\text{max}} \) is between 500 and 1000 A/cm\(^2\), and the average ion energy \( E_0 = 350 \text{ keV} \) [4]. The choice of the ion current density \( j_1(t) \) in Eq. (1.3) derives from the requirement that the total energy transferred from the ion beam to the target during the pulse (total energy is proportional to \( j_{\text{max}} \tau/2 \)) be the same for all functions \( j_i(t) \). When \( j(t) = \text{const} \) the source is a step in both time and in the coordinate \( x \) (normal to the surface). This corresponds to a uniform distribution of power \( (E_0 j) \) in the beam, and to a uniform energy distribution for the ions. The functions \( j_i(t) \) are shown in Fig. 1.

We should point out that, in our model, we take into account the temperature dependence of the kinetic coefficients \( a \) and \( c \). The thermal conductivity \( a \) is approximated by a third-order polynomial up to the melting temperature:

\[
a(t) = a_0 + a_1(T - T_0) + a_2(T - T_0)^2 + a_3(T - T_0)^3
\]

and the numerical values of the coefficients \( a_i \) are determined from the known values of the thermal conductivity at different temperatures taken from a handbook [5]. The value of \( a_0 \) is the thermal conductivity at \( T_0 = 20^\circ \text{C} \). The thermal conductivity can be assumed constant only for small temperature changes. The solution to Eq. (1.1) is well known [6, 7] when the parameters are constants. For example, the solution to the one-dimensional problem of an instantaneous planar heat source that deposits the energy \( E_0 = c p Q_0 \) per unit area at time zero in the plane \( x = 0 \) is

\[
T(x, 0) = 0
\]

and for nonzero \( x \) has this form