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# MODELING OF ION BEAM SURFACE TREATMENT

R. W. Stinnett, Quantum Manufacturing Technologies, Inc.
3701 Hawkins St. NE
Albuquerque, NM

J. E. Maenchen and T. J. Renk, Sandia National Laboratories
Albuquerque, NM 87185

K. W. Struve, Mission Research Corporation
Albuquerque, NM

Mark M. Campbell, PASTDCO
1248 Princeton NE
Albuquerque, NM 87106

**Abstract**

*The use of intense pulsed ion beams is providing a new capability for surface engineering based on rapid thermal processing of the top few microns of metal, ceramic, and glass surfaces. The Ion Beam Surface Treatment (IBEST) process has been shown to produce enhancements in the hardness, corrosion, wear, and fatigue properties of surfaces by rapid melt and resolidification. We have created a new code called IBMOD that enables the modeling of intense ion beam deposition and the resulting rapid thermal cycling of surfaces. This code has been used to model the effect of treatment of aluminum, iron, and titanium using different ion species and pulse durations.*

## 1. Introduction

The emerging capability to produce high average power (5-100 kW) pulsed ion beams at 0.1-1 MeV energies is enabling the development of a new, commercial scale thermal surface treatment technology called Ion Beam Surface Treatment[1] (IBEST). IBEST uses high energy pulsed (0.03-1μs) ion beams to directly deposit energy in the top 0.1-10 micrometers of the surface of materials, including metals, ceramics, and glass. This is illustrated in Figure 1. The depth of treatment is controllable by varying the ion energy and species. Efficient deposition of the energy in a thin surface layer allows melting of the layer with relatively small energies ( typically 1-10 J/cm$^2$) and allows rapid cooling and resolidification of the melted layer by thermal diffusion into the underlying substrate. Typical cooling rates (>1x10$^9$ K/sec) are sufficient to cause amorphous and fine grain layer formation and the production of new microstructures including nano-crystalline and metastable phases. IBEST has been used to melt and resolidify metals, glass and ceramics for a variety of possible industrial applications. Experiments have shown that surfaces treated by this rapid quenching technique can have significantly improved properties that depend on the specific material but include corrosion, wear, and hardness and the production of smooth and crack-free surfaces.

Because the effects of IBEST on materials are based on rapid thermal cycling, the capability to model this thermal cycling is crucial to the understanding and application of IBEST to different materials and geometries. We have developed a new code called IBMOD that is specifically designed to model IBEST processing. IBMOD calculates the deposition of ions in materials and follows the resulting temperature variation with time and one dimensional spatial resolution. IBMOD is based on the RANGE code originally developed at Sandia National Laboratories by J. Maenchen. It provides the capability to use different pulse shapes and durations, multiple ion species, time varying ion energies, varying beam incidence angles, and temperature-dependent materials properties.



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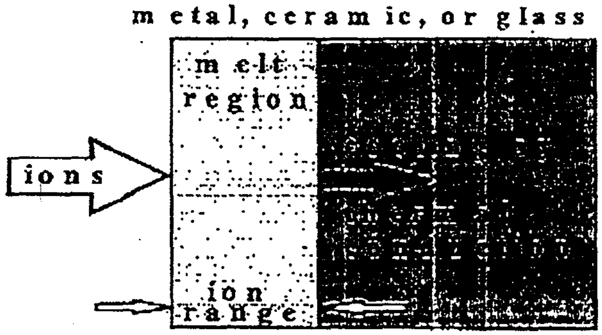


Figure 1. The Ion Beam Surface Treatment process uses short (<1μs), intense pulses of ions to melt surfaces. This melting is followed by rapid resolidification at $10^9$K/s. The IBMOD code models this process with time and one dimensional spatial resolution.

## 2. IBMOD Code Description

IBMOD is an outgrowth of the RANGE code developed by J. Maenchen at Sandia National Laboratories. IBMOD combines energy deposition based on the Anderson and Ziegler formulations[2] with thermal relaxation using a 1-D fully implicit, finite difference algorithm[3] that has been modified to include a time-dependent source, variable spatial zoning, temperature dependent specific heat and thermal conductivity and melting/resolidification phase transitions. The stopping powers used in IBMOD includes zeroth order corrections to the electron energy loss to account for straggling.

Because of the short time scale characteristic of IBEST, IBMOD allows superheating of the liquid surface layer above the equilibrium vapor temperature. The temperature is clamped when it reaches the ablation temperature[4], given by $T_{ablation} = 0.1H_v/R$, where $H_v$ is the heat of vaporization and R is the universal gas constant.

IBMOD can model deposition using user-specified ion species as well as ion energy and current density profiles. Multiple ion species with different time histories can also be used. It is also possible to model multiple layers of different materials.

Temperature dependent data for over 30 materials including elements, alloys, ceramics, glasses, and polymers is already available in IBMOD. Calculations indicate the inclusion of temperature dependent specific heat and thermal conductivity data is important for accurate IBEST modeling and typically changes calculated peak temperatures by 15-30%.

## 3. Modeling Results

In order to explore the modeling capability of IBMOD we have used the simple but representative ion voltage and current waveforms shown in Tables 1 and 2. The energy density delivered to the surface in either case is 4.0 J/cm$^2$. Different energy densities were obtained by scaling the incident current densities. The results of aluminum surface treatment with hydrogen ions and carbon ions, using pulse lengths of 180 ns and 1000 ns are shown in Figures 2,3, and 4.

Table 1. Ion voltage and current density waveforms used for the 180 ns, 4J/cm$^2$ case.

| Time - ns | Voltage-kV | Current Density-A/cm2 |
|---|---|---|
| 0 | 400 | 58.5 |
| 180 | 300 | 70.0 |
| 181 | 0 | 0 |

Table 2. Ion voltage and current density waveforms used for the 1000 ns, 4 J/cm$^2$ case.

| Time - ns | Voltage-kV | Current Density-A/cm2 |
|---|---|---|
| 0 | 400 | 10.5 |
| 1000 | 300 | 12.6 |
| 1001 | 0 | 0 |

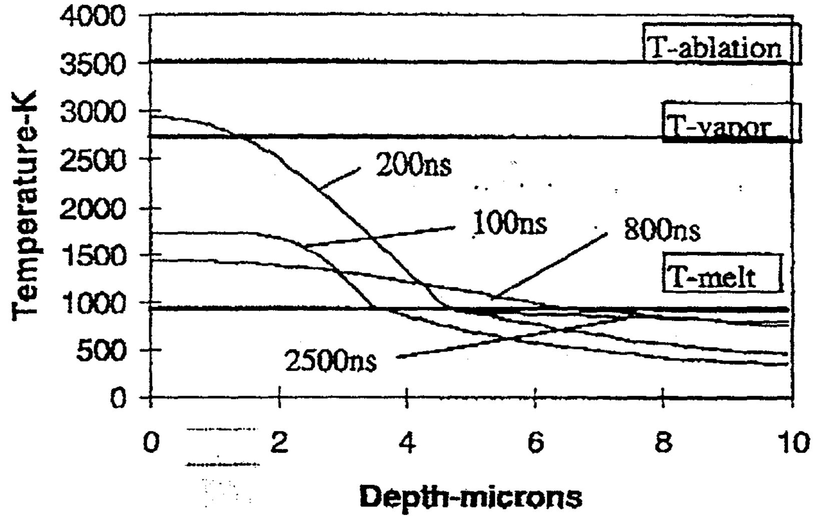


Figure 2. Temperature as a function of time and depth in an aluminum sample treated using a 4 $J/cm^2$ proton beam as described in table 1. The treatment level was chosen to not significantly exceed the vapor temperature for aluminum.

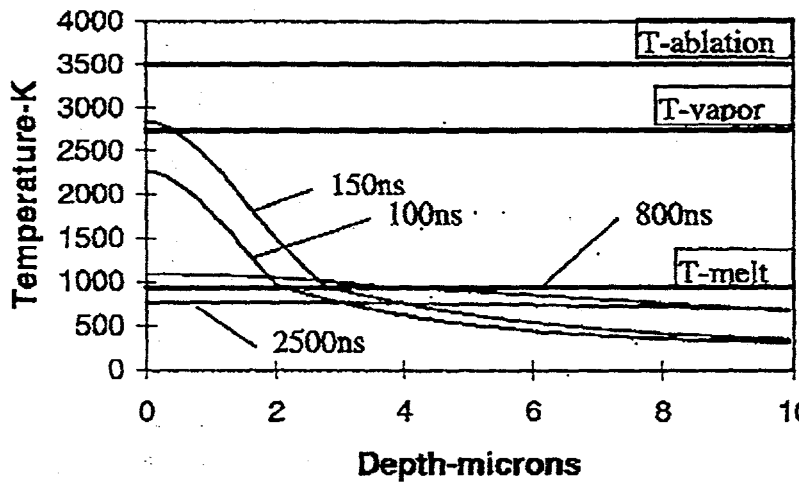


Figure 3. Temperature as a function of time and depth in an aluminum sample treated using a 2.8 $J/cm^2$ carbon (+1) ion beam with the waveshape described in table 1 but with current densities scaled down by 30% to limit the peak temperature to that shown in Figure 2.

Although the metrics for optimum IBEST processing are still being determined, it is likely that optimum treatment will result from the energy efficient achievement of the maximum temperature possible over the maximum depth obtainable without ablating the surface. Figure 2 predicts that a temperature of 2500-3000K in a 2 micron depth of aluminum can be achieved using a 4$J/cm^2$, 180 ns pulse of 300-400 kV protons. The total melt depth is 6.5 microns.

Figure 3 shows that the use of carbon ions instead of protons causes the energy to be deposited nearer the surface, resulting in a more surface-peaked temperature profile and limits the amount of energy that can be deposited without exceeding the vapor temperature to 2.8 $J/cm^2$. This reduces the depth that can be heated to 2500-3000K to less than 1 micron. The total melt depth is 4 microns.

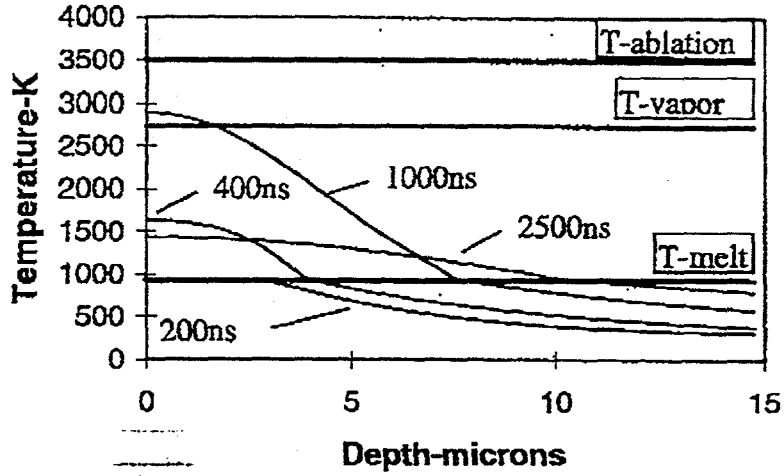


Figure 4. Temperature as a function of time and depth in an aluminum sample treated using a 6.8 J/cm$^2$ proton beam with the waveshape described in table 2 but with current densities scaled up by 70% to achieve the same peak temperature as the cases shown in Figures 2 and 3.

The use of a 1000 ns long proton pulse, as shown in Figure 4, requires 70% more energy to achieve 2500-3000K temperature over a 2 micron depth because of the increased effect of thermal conduction. The greater energy does, however, result in a 10 micron melt depth.

**Discussion**

These calculations illustrate the effects of different ion species and pulse lengths on the treatment of aluminum. Calculations for iron and titanium show similar effects. Process development and optimization for a variety of materials is now being done on Sandia National Laboratories' RHEPP-1 facility. IBMOD has successfully modeled observed melt depths in initial tests with aluminum and steel. It will be extensively used in the future to correlate time and depth resolved temperature profiles with experimentally measured enhancements in surface properties. Additional tests are planned to further verify the ability of IBMOD to accurately model a range of treatment parameters and materials of interest in surface engineering applications.

The new modeling capability provided by IBMOD will be an essential tool in understanding and developing optimum IBEST processing parameters for a range of materials and applications.

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