

LA-UR-04- 7811

Approved for public release;  
distribution is unlimited.

*Title:* MODELING OF THE THERMAL RESPONSE OF  
ION-TREATED MATERIALS

*Author(s):* ROBERT R. PETERSON

*Submitted to:* ANNUAL MEETING OF THE AMERICAN PHYSICAL  
SOCIETY DIVISION OF PLASMA PHYSICS  
NOVEMBER 15-19, 2004  
SAVANNAH, GA



Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by the University of California for the U.S. Department of Energy under contract W-7405-ENG-36. By acceptance of this article, the publisher recognizes that the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.

Form 836 (8/00)



# Modeling of the Thermal Response of Ion-Treated Materials

Robert R. Peterson

Los Alamos National Laboratory

Annual Meeting of the  
American Physical Society Division of Plasma Physics  
November 15-18, 2004  
Savannah, GA

Mini-conference on Ion Treatment of Materials



*X-1 Plasma Physics  
Applied Physics Division*

RRP  
Ion Treatment



P 1

# ABSTRACT

The RHEPP facility at Sandia National Laboratories offers an excellent experimental environment to study the rapid ion beam heating of materials. Its ion beams are able to create surface temperatures in materials of interest that are at or above the melting temperature with temperature gradients that can create plastic flow. These conditions lead to the formation of surface roughness in some materials but not in others. The BUCKY computer code can model the deposition of ion beams, the resulting energy transport, and the induced motion of the sample in one-dimension. The key to proper modeling of these experiments is stress/strain response at temperatures just below melting. Here the stresses induced by temperature gradients are can cause plastic strain in the material. Pure hydrodynamic calculations are not adequate to model these phenomena, because the Euler equations and energy equations must include the effects of stress. Phenomenological equations of state and strength properties that are calibrated to known properties of materials are being added to BUCKY. It is particularly important that the effect of strain rate on the material strength is included. This approach is being investigated in the modeling with BUCKY of RHEPP experiments on Tungsten and Titanium.

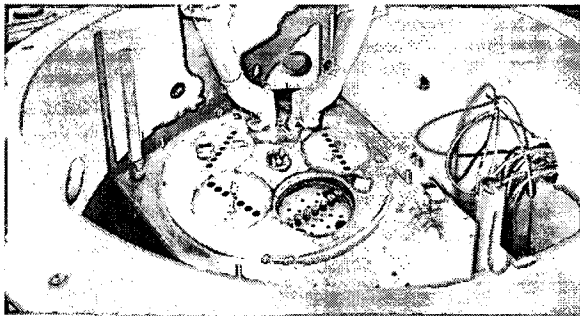


# OUTLINE

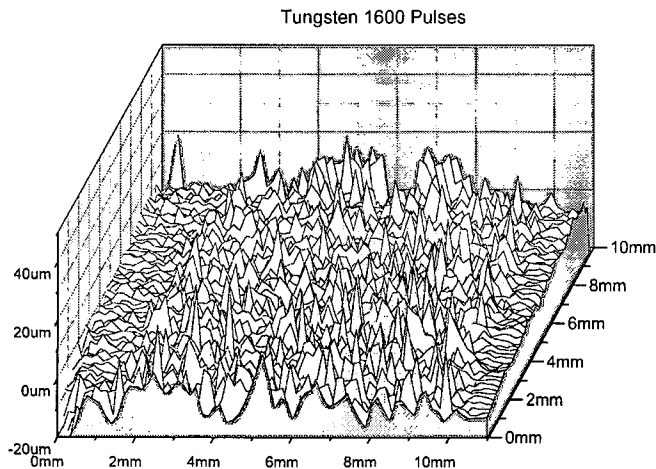
- BUCKY Code
- Energy Deposition
- Heat Transport
- Phase Changes
- Material Strength and Yielding



# Why do RHEPP Treated Materials Roughen?



- Occurs in some materials (W) and not in others (Al).
- Occurs below vaporization and melting thresholds.
- Hypothesis: Roughening is due to thermal stresses and yielding.
- Modeled with BUCKY Code



# BUCKY Computer Code

- Lagrangian Radiation Hydrodynamics Code
- Models RHEPP Experiments
- Detailed Ion Deposition
- Plasma Region; radiation transport, Spitzer conductivity, hydro-motion
- Solid/Liquid Region; instantaneous x-ray deposition only, tabulated measured conductivities, no hydro.
- Stress and Yielding Post-processed.

# Energy Deposition

- Energy and Time-Dependent Ion Deposition

Stopping Power

Projectile Charge State

$$S = \frac{1}{N_{bg}} \left[ \left( \frac{dE}{dx} \right)_{fe} + \left( \frac{dE}{dx} \right)_{be} + \left( \frac{dE}{dx} \right)_{nucl} \right] \quad \frac{dN_q}{dt} = -N_q (n_e C_q + n_e^2 \alpha_q^{coll} + n_e \alpha_q^{rad} + N_{bg} v, \sigma_{cx,q})$$

$$\left( \frac{dE}{dx} \right)_{fe} = \left( \frac{\omega_p q_1 e}{v_1} \right)^2 G(y^2) \ln \Lambda_{fe} \quad G(y^2) = erf(y) - \frac{2}{\sqrt{\pi}} e^{-y^2} \quad y = \frac{v_p}{\langle v_e \rangle}$$

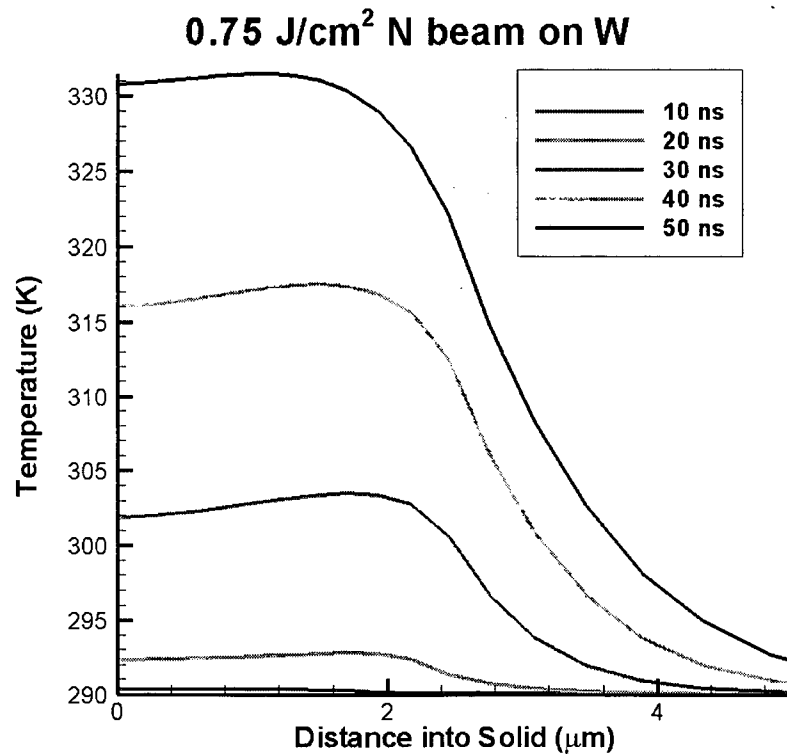
$$\left( \frac{dE}{dx} \right)_{nucl} = C_1 \varepsilon^{1/2} \exp \left\{ -45.2 (C_2 \varepsilon)^{0.277} \right\} \quad \varepsilon = E / A_1 (MeV / amu)$$

$$\left( \frac{dE}{dx} \right)_{be} = \begin{cases} \left( \frac{dE}{dx} \right)_{LS} & v_1 < v_L \\ (1-f) \left( \frac{dE}{dx} \right)_{LS} + f \left( \frac{dE}{dx} \right)_{Bethe} & v_L \leq v_1 \leq v_b \\ \left( \frac{dE}{dx} \right)_{Bethe} & v_1 < v_B \end{cases} \quad \left( \frac{dE}{dx} \right)_{LS} = (3.84 \times 10^{18} keVcm^{-1}) N_2 \frac{Z_1^{7/6} Z_2^*}{[Z_1^{2/3} + (Z_2^*)^{2/3}]^{3/2}} \left( \frac{E_1}{A_1} \right)^{1/2}$$

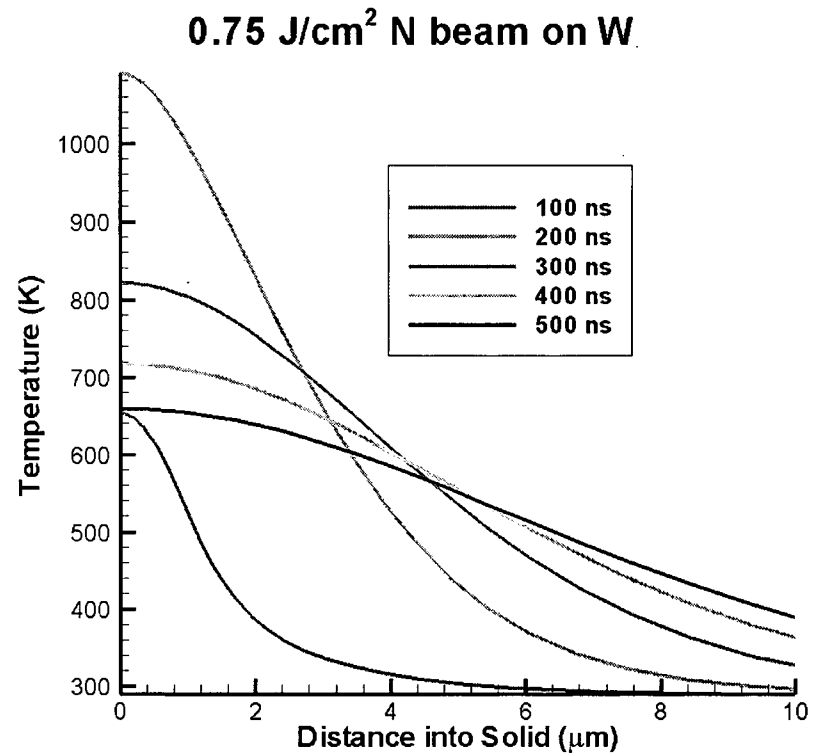
$$\left( \frac{dE}{dx} \right)_{Bethe} = \left( \frac{\omega_p q_1 e}{v_1} \right) \left[ \ln \left[ \frac{2m_e v_1^2}{\langle \Phi_2 \rangle (1 - V_1^2 / c^2)} \right] - \left( \frac{v_1}{c} \right)^2 \right]$$

# Energy Deposition Example

Early times show deposition peaks



Late times show deposition peaks washed out by conduction



# Energy Transport

- Thermal Diffusion

Two Temperature Plasma with Hydro

$$C_{ve} \frac{\partial T_e}{\partial t} = \frac{\partial}{\partial m_o} \left( r^{\delta-1} K_e \frac{\partial T_e}{\partial r} \right) - \omega_c (T_e - T_i) - \left[ (E_e)_v + P_e \right] \frac{\partial V}{\partial t} T_e + A - J + S_e$$

One Temperature Solid or Liquid without Hydro

$$Cp \frac{dT}{dt} = \frac{\kappa}{\rho} \frac{d^2 T}{dx^2} + S$$

- Radiation Transport (only in Plasma)

$$V \frac{\partial E_R^g}{\partial t} = \frac{\partial}{\partial m_o} \left( r^{\delta-1} K_R^g \frac{\partial E_R^g}{\partial r} \right) - \frac{4}{3} E_R^g \dot{V} - c \sigma_{P,A}^g E_R^g + J^g, \quad g = 1, \dots, G$$

# Temperature Dependant Conductivities

- Spitzer is the standard in BUCKY

$$K_e = 20 \left( \frac{2}{\pi} \right)^{3/2} \frac{(k_B T_e)^{5/2} k_B \epsilon \delta_T}{m_e^{1/2} e^4 Z \ln \Lambda_{ei}} \quad \epsilon \delta_T = \frac{0.43Z}{(3.44 + Z + 0.26 \ln Z)}$$

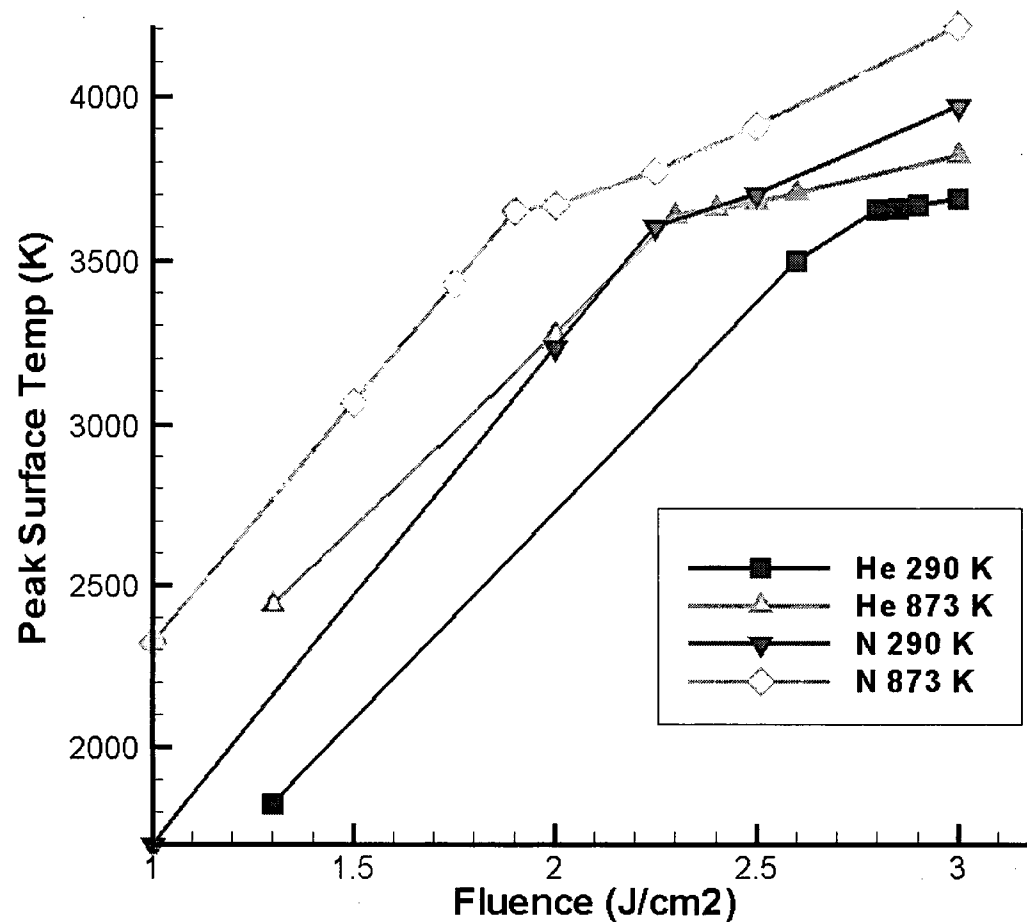
- Tabulated Temperature-Dependent Conductivities are Better for Solids

$$C_p \frac{dT}{dt} = \frac{\kappa}{\rho} \frac{d^2 T}{dx^2} + S$$

$\kappa = \kappa(T)$  from table

$C_p = C_p(T)$  from table

# Energy Transport Example



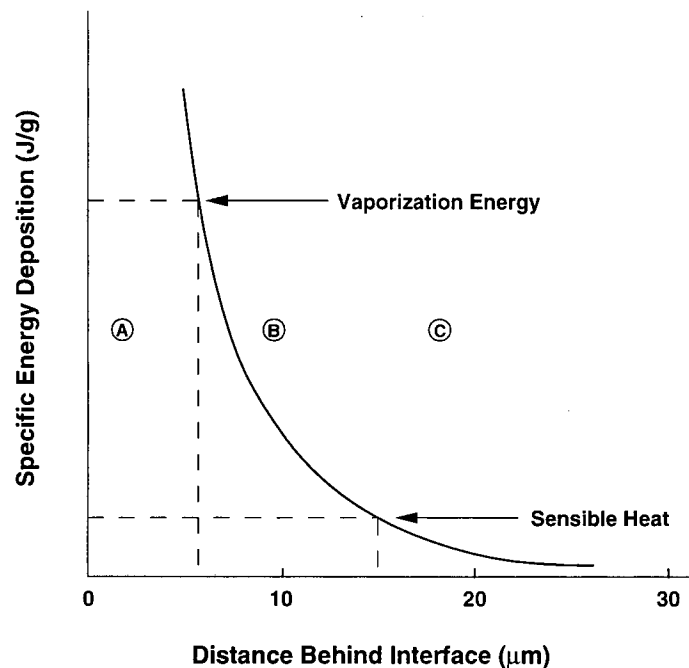
Change in slope noted when melting starts

# Phase Changes

- Phase Changes lead to measurable modification of materials (roughening of tungsten?)
- Vaporization removes material and applies a recoil impulse.
- Melting leaves a layer with a different grain structure.
- Both remove substantial energy in latent heat.

# Vaporization

## Instantaneous Vaporization



## Continuous Vaporization and Condensation

$$(dm / dt)_v = \frac{2}{3} P_{sat} A_{wall} \left( \frac{\mu}{RT_v} \right)^{1/2}$$

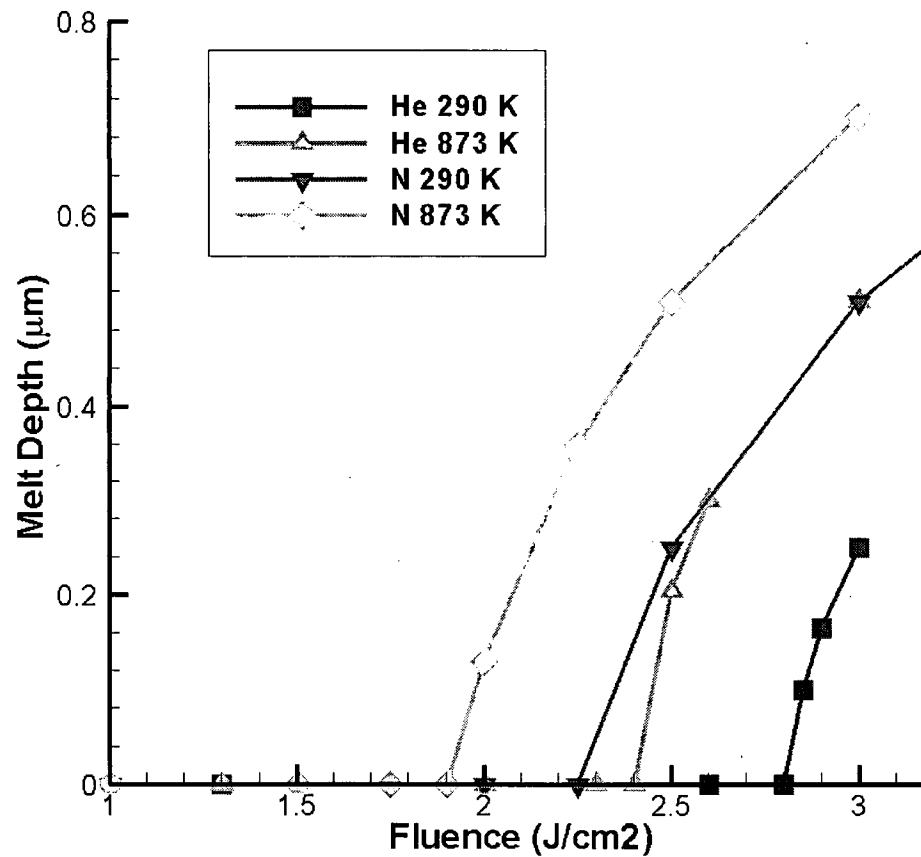
$$P_{sat} = \exp \left\{ \frac{\Delta H_v}{kT_{vap,o}} \left( 1 - \frac{T_{vap,o}}{T_c} \right) \right\} bar.$$

$$(dm / dt)_c = \frac{2}{3} f_s f_{NC} P_{vap} A_{wall} \left( \frac{\mu}{RT_v} \right)^{1/2}$$

# Melting

- Melting needs to include accounting for the heat of fusion,  $\Delta H_f$ .
- In BUCKY,  $\Delta H_f/T_{\text{melt}}$  is added to  $C_p$  in region around  $T_{\text{melt}}$ .

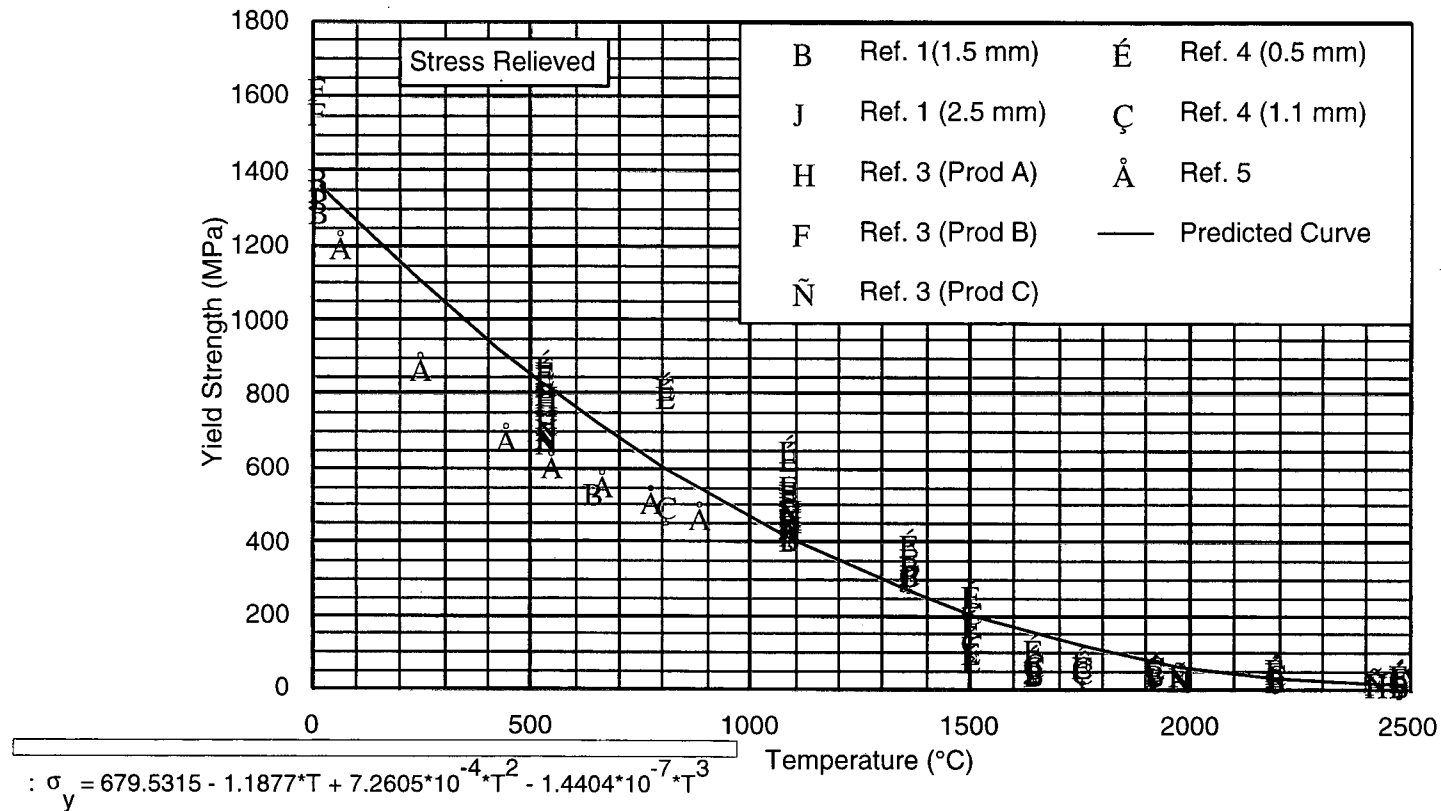
# Phase Change Example



# Material Strength and Yielding

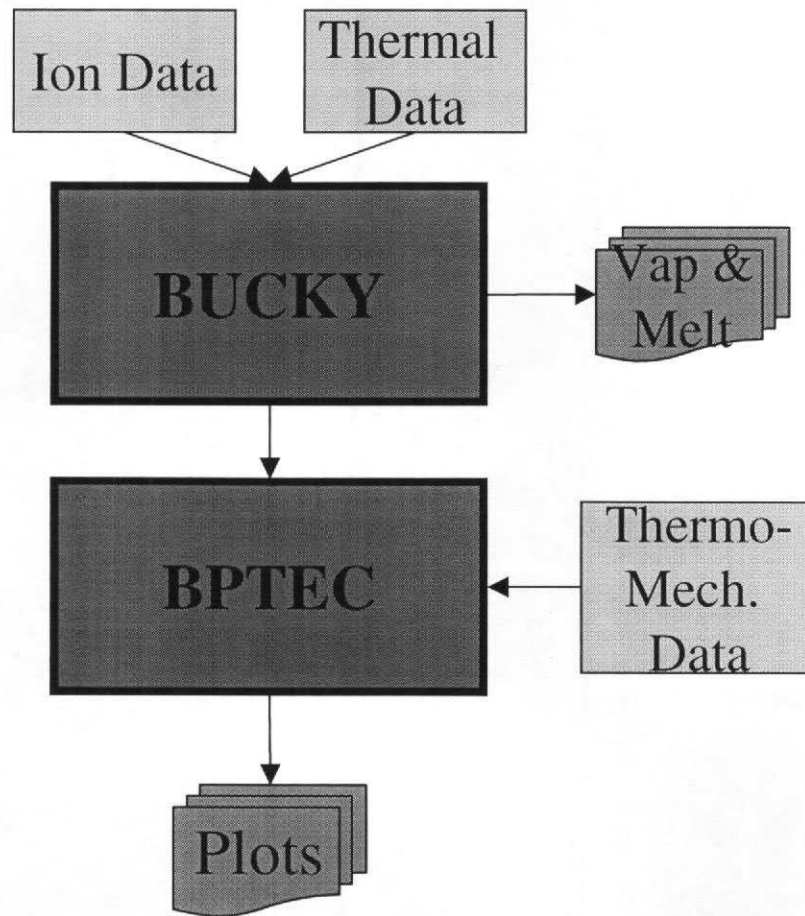
- The material ( $W$  in the RHEPP experiments of interest) can experience strong thermal gradients, leading to thermal stresses.
- Even when the surface does not melt, the surface temperature can be close to melting so the yield stress is very low.
- So the region near the surface is clearly yielding.
- BUCKY presently models this via post-processing (i.e. no plastic flow).

# Yield Strength is Reduced a High Temperatures



Ref: J. W. Davis (US), V. Barabash (JCT/RF), and S. Fabritsiev (RF) ITER Materials Properties Handbook.

# A Simple Way to Estimate the Onset of Yielding



- Ion Data: from SNL
- Thermal Data:  $\kappa(T)$ ,  $C_p(T)$ ,  $\Delta H_v$ ,  $\Delta H_m$

- Elastic Stress Model.
- Temperature-dependent Data for  $W$  from ITER manual.

$$\sigma = \frac{E \alpha (T - T_{ref})}{(1 - \nu)}$$

# Plastic Flow in Hydro-Codes

- Near the surface of tungsten in many RHEPP experiments, the thermal stresses would substantially exceed the yield stress if the material did not flow to relieve this stress.
- Therefore, plastic flow needs to be included in a complete model of these experiments.
- BUCKY does not have such a treatment, but some rad-hydro codes do. What follows is a discussion of possible methods.

# Plastic Flow Models

- Pressure Threshold:

$$\frac{\partial u}{\partial t} = -\frac{1}{\rho} \frac{\partial}{\partial r} (P+q) \quad \begin{cases} P = P & \text{if } P \geq \sigma_y \\ P = 0 & \text{if } P < \sigma_y \end{cases}$$

- Elastic and Plastic Regimes:

Hooke's Law in Elastic Regime and  $\frac{\partial u}{\partial t} = -\frac{1}{\rho} \frac{\partial}{\partial r} (P+q)$  In Plastic

- Greuneisen EOS:

$$P - P_H = \rho \gamma (E - E_H)$$

# The Mie-Grueneisen EOS

Taken from D.S. Lemons and C.M. Lund, "Thermodynamics of High Temperature Mie-Grueneisen Solid", *Am., J. Phys.* **67**, 1105 (1999).

$$P = \frac{\Gamma C_v T}{V} + \frac{3c_s^2}{(n-m)V_0} \left[ \left( \frac{V_0}{V} \right)^{n/3+1} - \left( \frac{V_0}{V} \right)^{m/3+1} \right]$$

$$E = C_v T + \frac{9c_s^2}{(n-m)} \left[ \frac{1}{n} \left( \frac{V_0}{V} \right)^{n/3} - \frac{1}{m} \left( \frac{V_0}{V} \right)^{m/3} - \frac{1}{n} + \frac{1}{m} \right]$$

Is a 6 parameter thermodynamically consistent EOS can be adjusted to capture tensile yield strength,

$$\sigma_y = - \left( \frac{3c_s^2}{V_0} \right) \frac{(m+3)^{\frac{m+3}{n-m}}}{(n+3)^{\frac{n+3}{n-m}}}$$

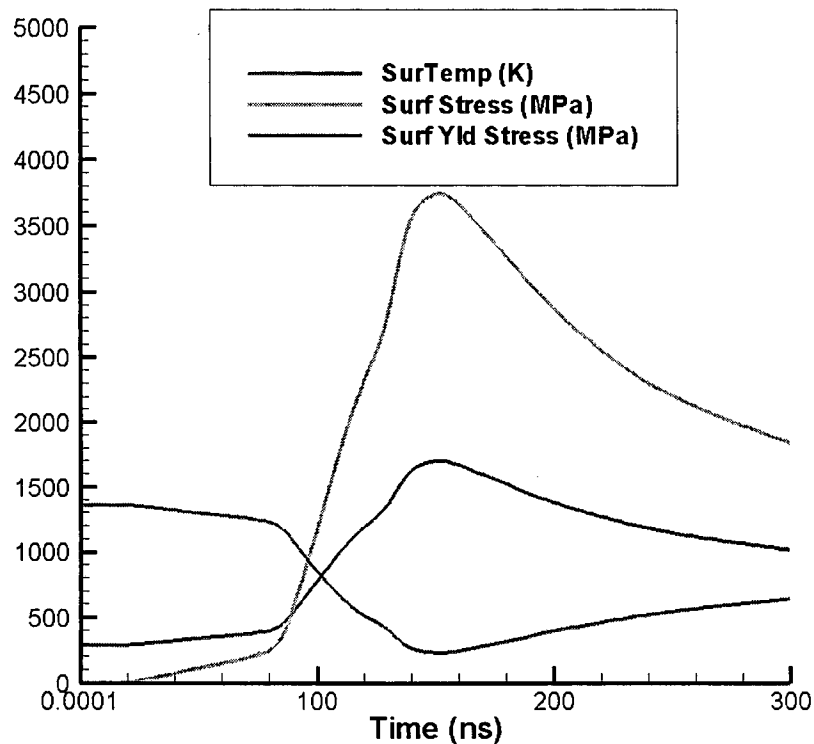
cohesive energy,

$$E_{coh} = \frac{9c_s^2}{nm}$$

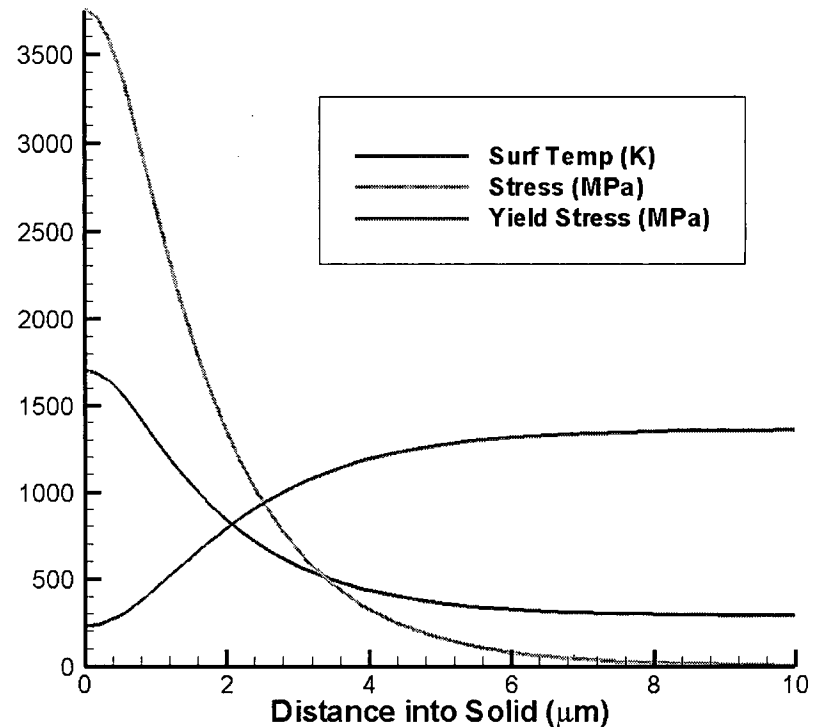
And normal density, specific heat, and speed of sound.  $\frac{1}{V_0}, C_v, c_s$

# Yielding Example

290 K Tungsten Irradiated by 1.0 J/cm<sup>2</sup> N Ion



290 K Tungsten Irradiated by 1.0 J/cm<sup>2</sup> N Ions Profile at 152 ns



# Conclusions

- Energy Deposition, Thermal Conduction, Vaporization and Melting all modeled with BUCKY
- Yielding via Post-processing; does not model plastic flow.
- Onset of yielding consistent with RHEPP experiments on Tungsten.
- Need to Add a Plastic Flow Model.