Stress and Yield Modeling in BUCKY

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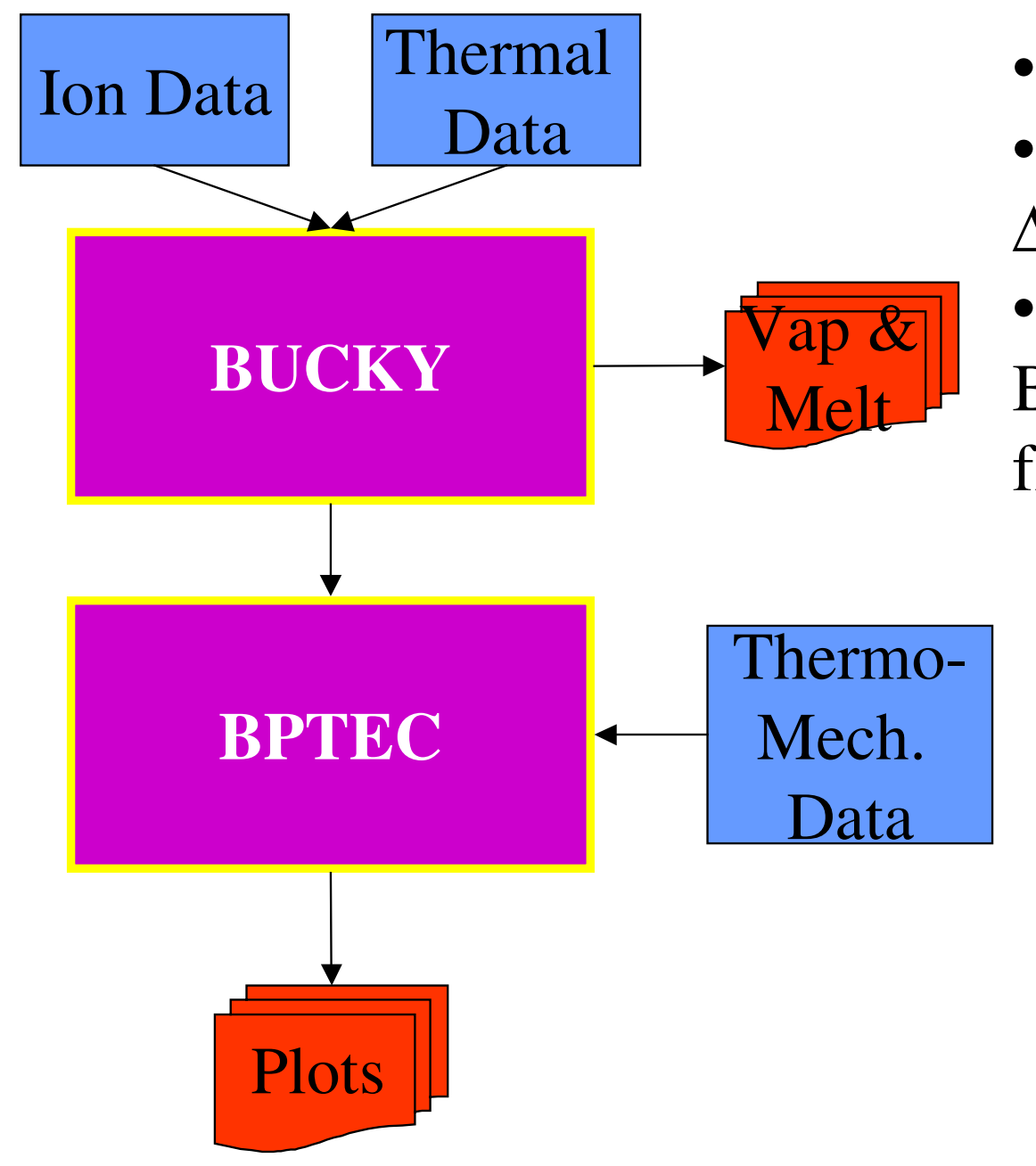
ABSTRACT

Calculations have been performed for experiments on the RHEPP accelerator at Sandia National Laboratories. RHEPP is a rep-rated pulsed power device and can repeatedly irradiate samples with pulses of a variety of ion types. The ion fluences per pulse range from 1 to 10 J/cm^2 and He and N ions are considered in the work reported here. BUCKY is a 1-D Lagrangian radiation hydrodynamics code developed at the University of Wisconsin, with ion deposition, heat transfer, melting, and vaporization. BUCKY output is post-processed to calculate elastic stresses. The BUCKY simulations show that the melting and stress behavior of the tungsten samples, irradiated by RHEPP, are affected by the ion species and the initial temperature of the sample. The calculations also show that, for all experiments performed in this series, there is substantial yielding in the surface layers of the tungsten. That helps to explain the surface roughening observed in the experiments below the melt fluence. This poster discusses current and future models for stresses in BUCKY. In particular, the Mie-Grueneisen equation of state and simple elastic models are discussed.

BUCKY Simulations Have Been Performed for RHEPP Experiments on Pure Tungsten at Different Initial Temperature and Ion Types

1. Melt threshold fluence and peak surface temperature depend on initial temperature and ion type (He or N).
2. Stress calculations performed for selected cases. All samples should exhibit yielding.
3. Plastic Flow Model: Mie-Grueneisen EOS.

Stress and Yield Post-Processing in BUCKY



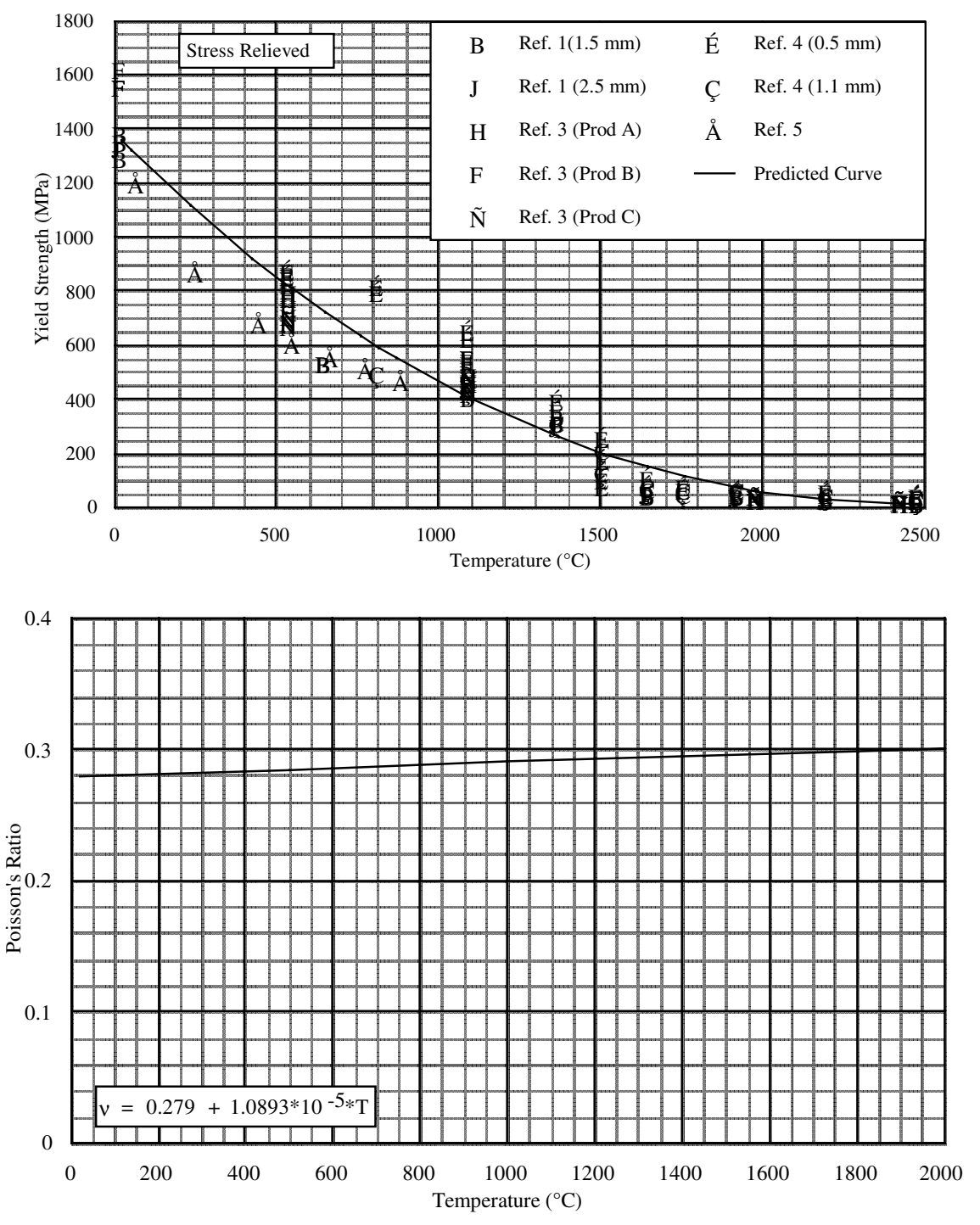
- Ion Data: from SNL
- Thermal Data: $\kappa(T)$, $C_p(T)$, ΔH_v, ΔH_m
- Mie-Grueneisen EOS is in BUCKY to model plastic flow.

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

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

Thermo-Mechanical Tungsten Data From ITER Materials Properties Handbook for BPTEC

$\sigma_y = 1384.617 - 1.2141*T + 3.1313*10^{-4}*T^2 - 1.8958*10^{-8}*T^3$
R0^2 = 0.9516

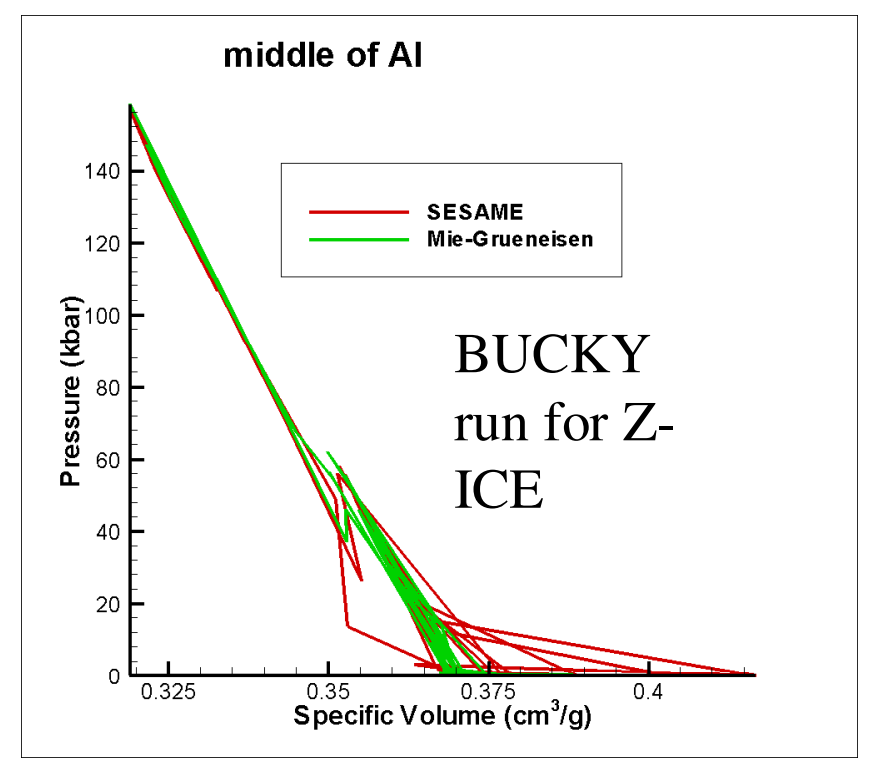


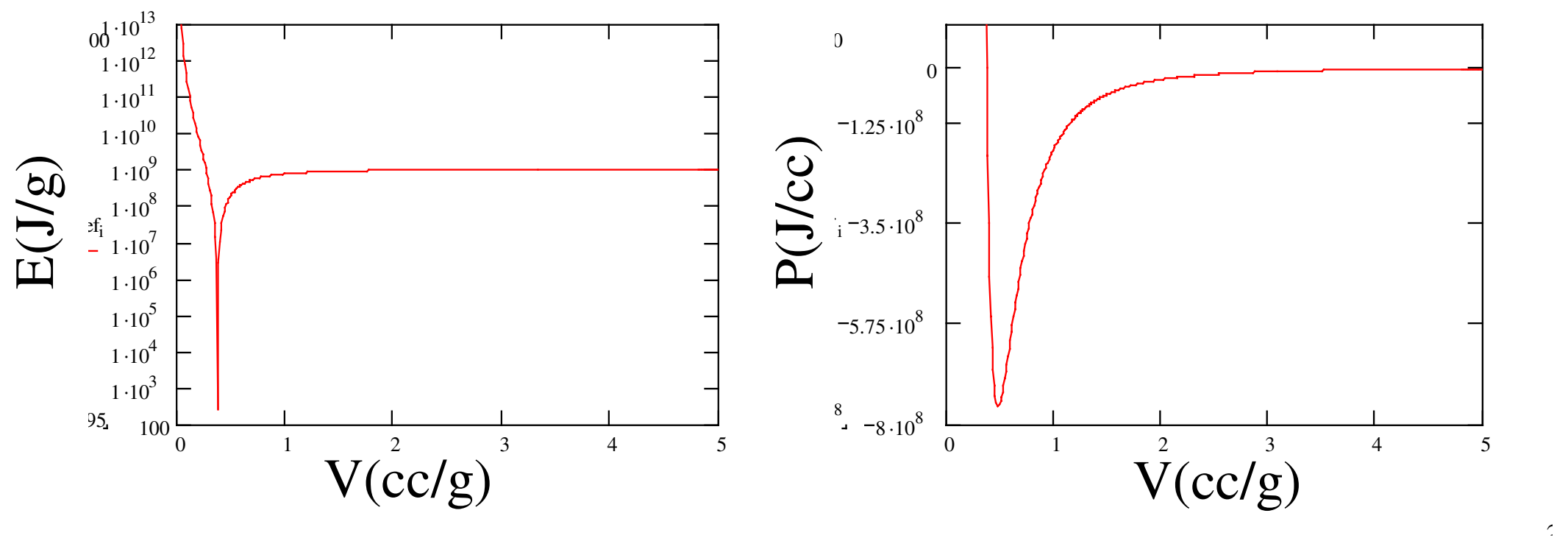
- Curves are only used up to a maximum temperature (different for each type of data) and are held constant at high T.
- The maximum temperature is well below melting.
- BUCKY/BPTEC calculations run to temperatures well beyond ends of curves, sometimes leading to odd behavior.

Sample for Aluminum from MATHCAD Program

SESAME uses Maxwell Construction
For these BUCKY runs minimum Pressure is 0.

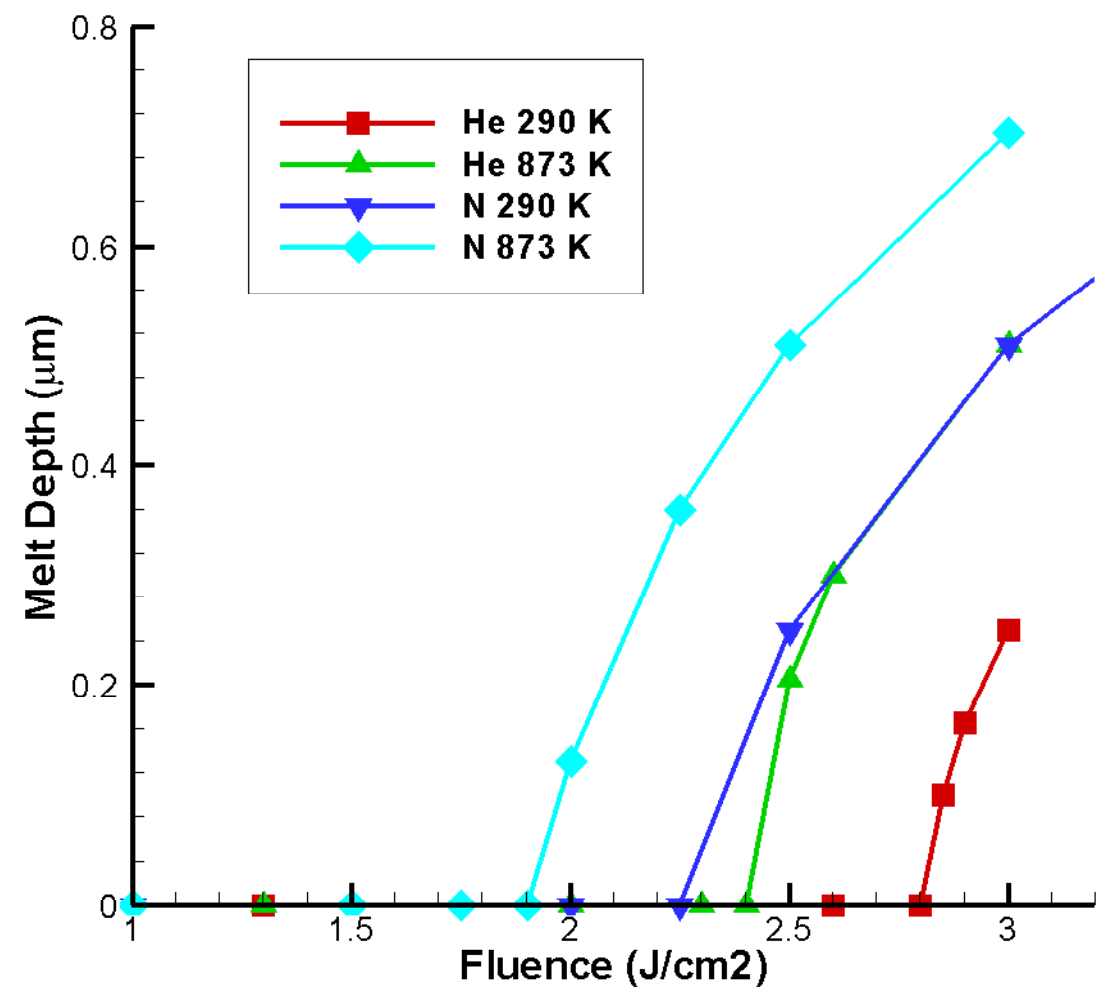
Γ=2.136
C_v=10,438 (J/gm-eV)
C_s=55,000 (cm/s)
V_0=0.37 (g/cm^3)
m=6
n=12





Melting Threshold Fluence is Sensitive to Ion Type and Initial Temperature

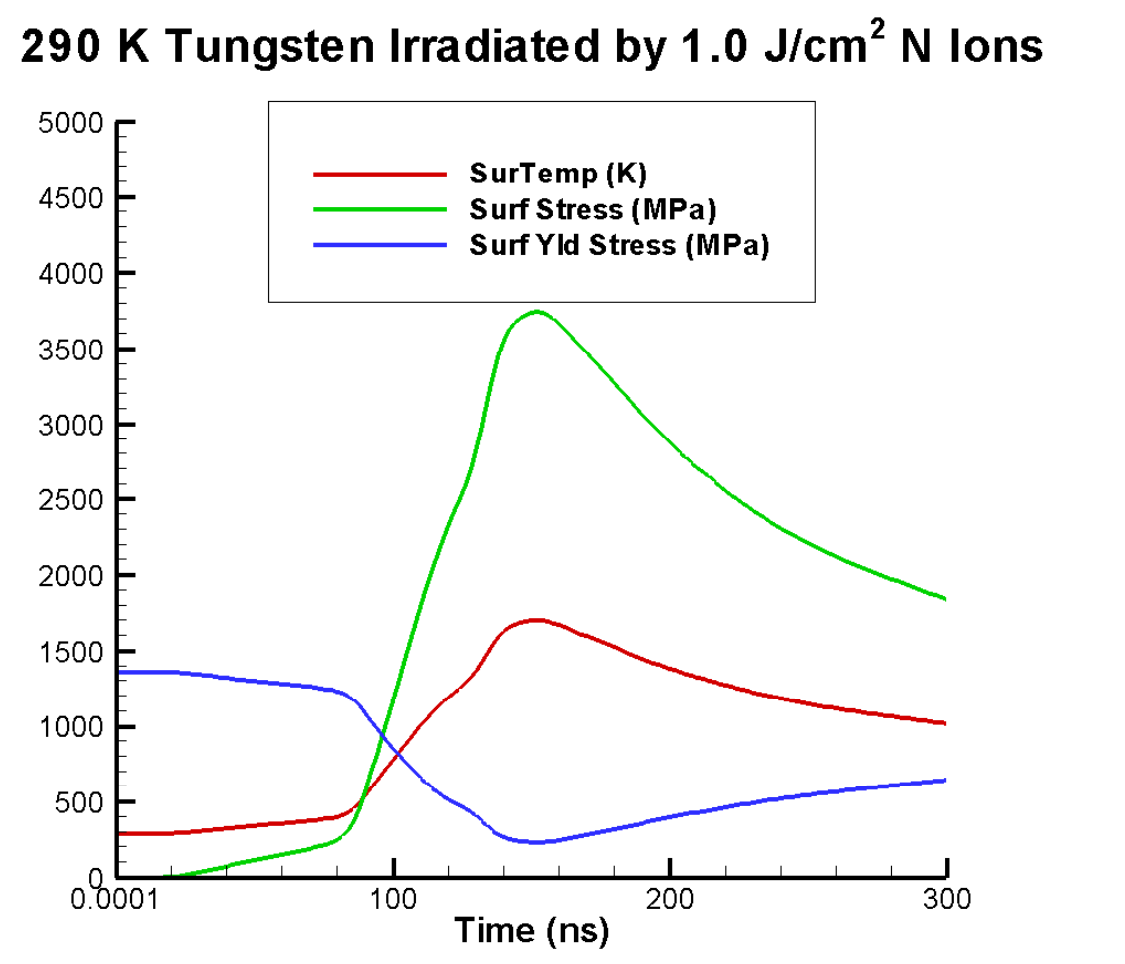
- Predicted RHEPP melting fluences vary between 1.9 and 2.8 J/cm^2.
- Tina Tanaka's thermal properties used for W.
- Pre-shot heating of the sample lowers melt threshold.
- A higher He fluence is required to melt W.

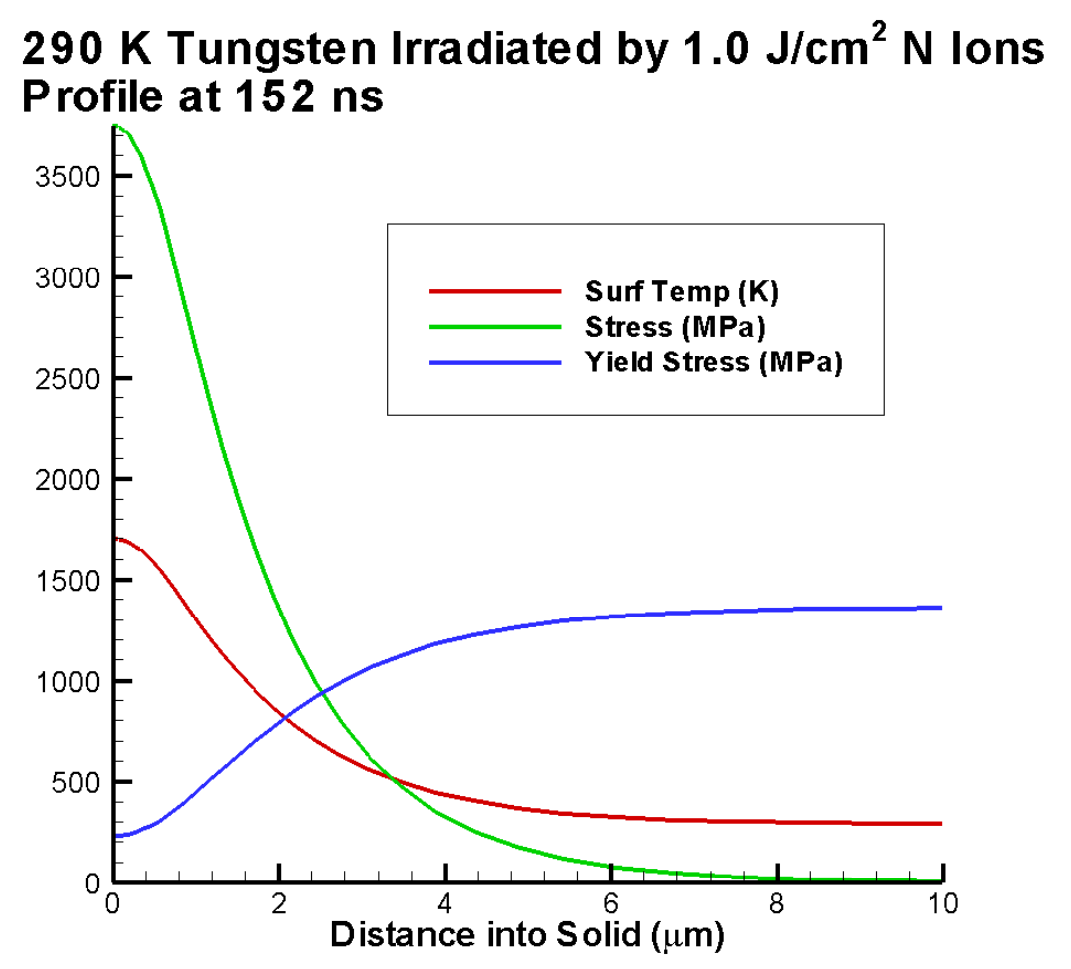


Least Damaged Case Still has Yielded Material

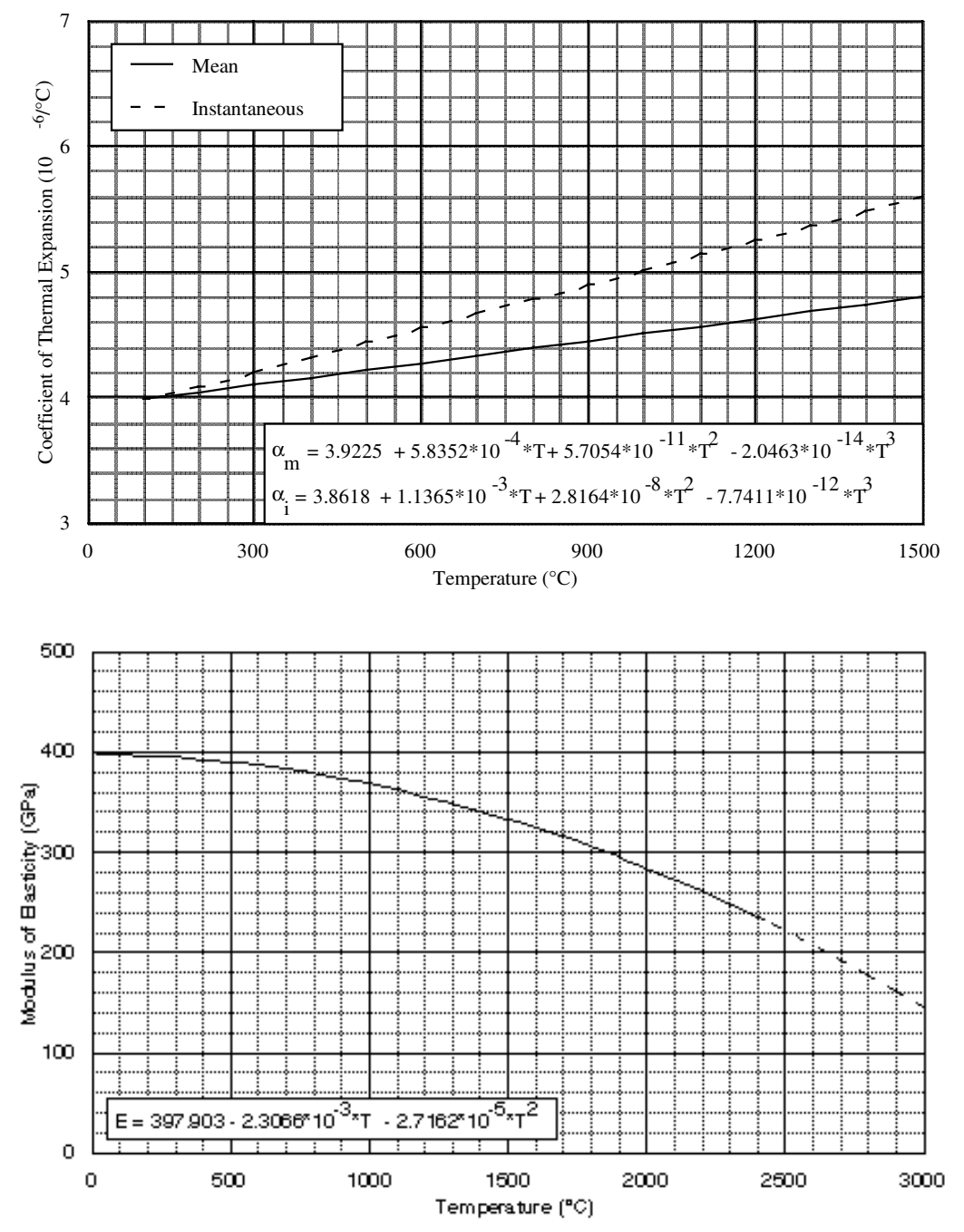
Yielding persists for more than 200 ns

At peak surface temperature, 2.5 μm of material is yielding

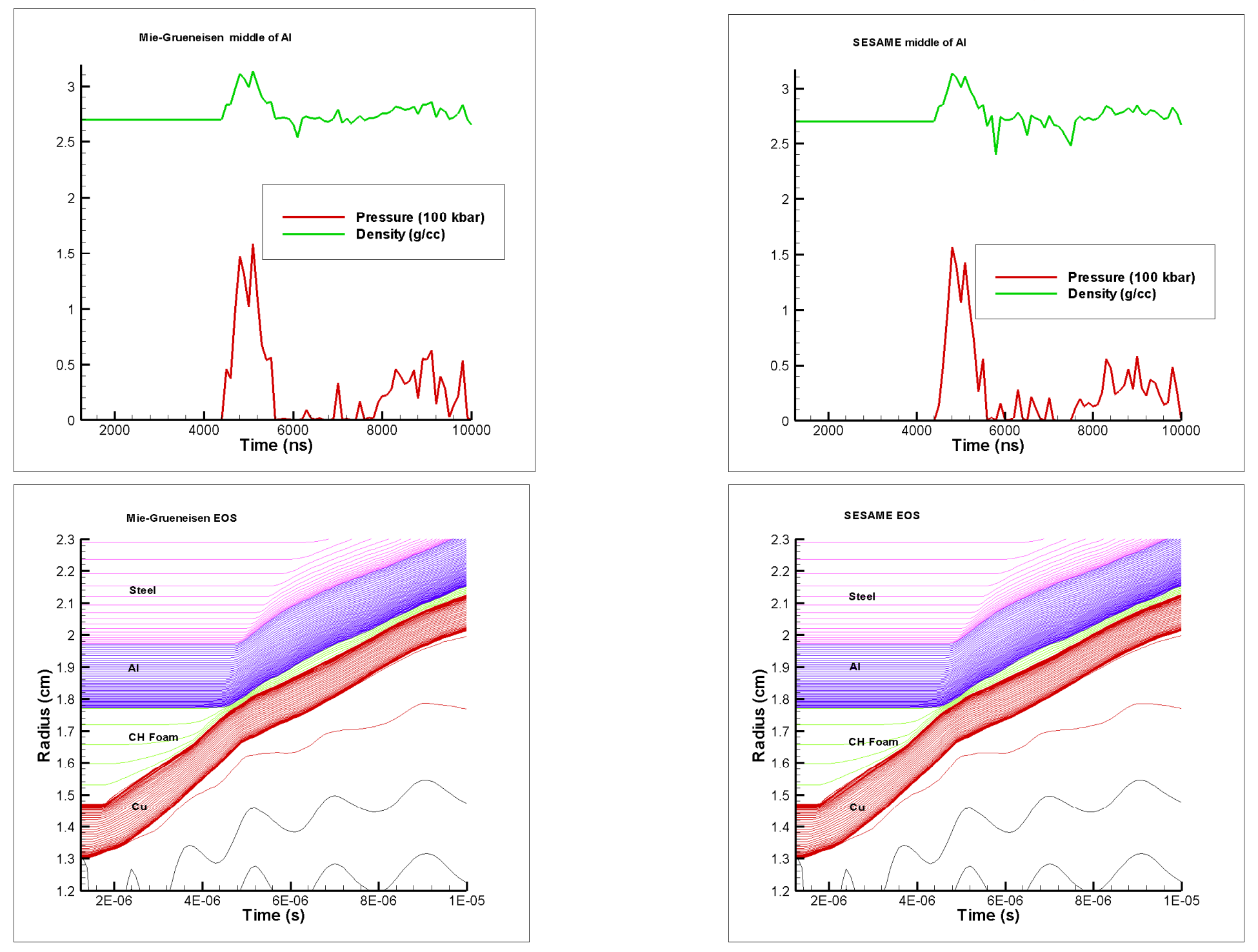




Thermo-Mechanical Tungsten Data From ITER Materials Properties Handbook For BPTEC

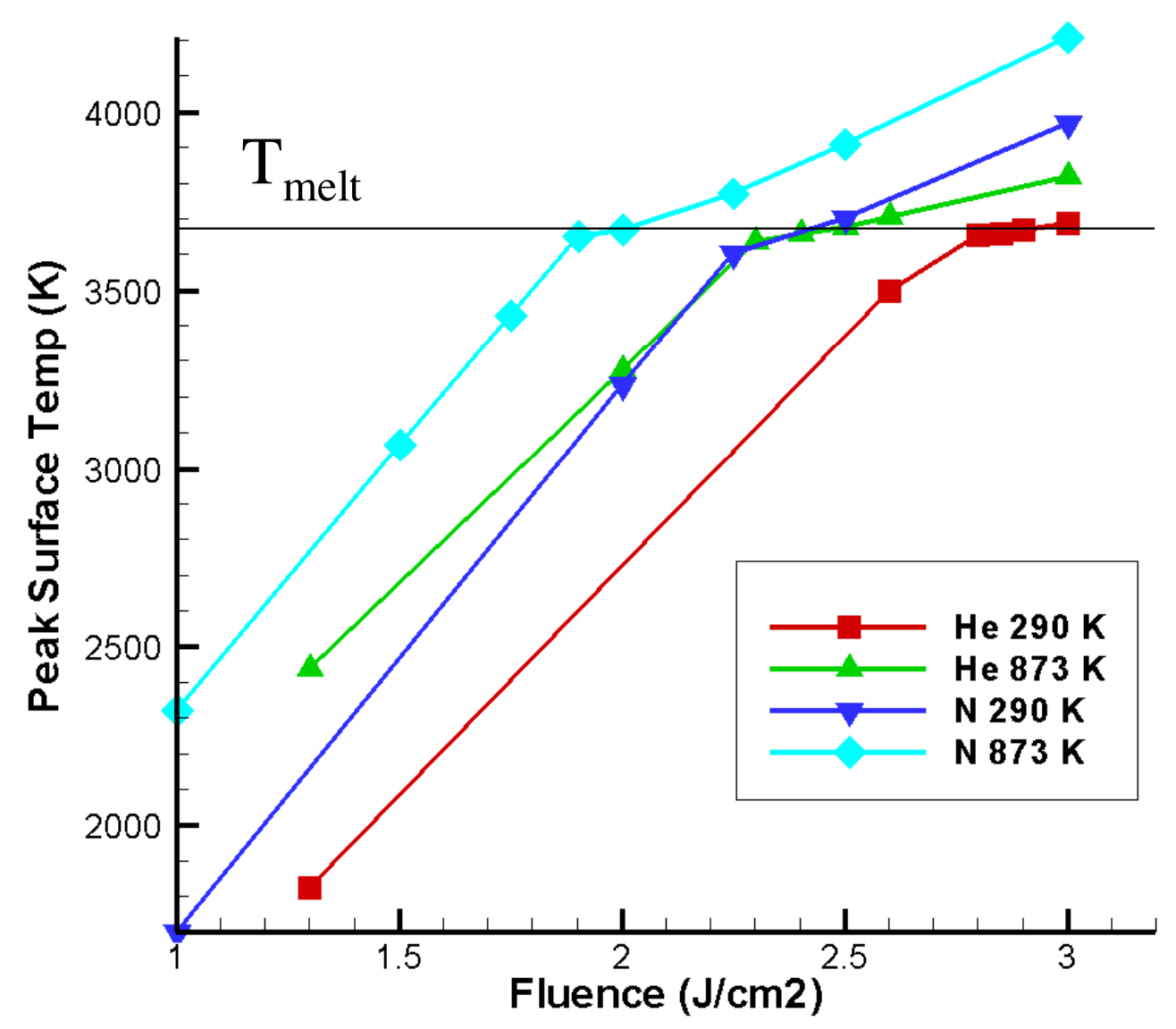


Z Isentropic Compression Experiment is a First Test of Mie-Grueneisen Model in BUCKY



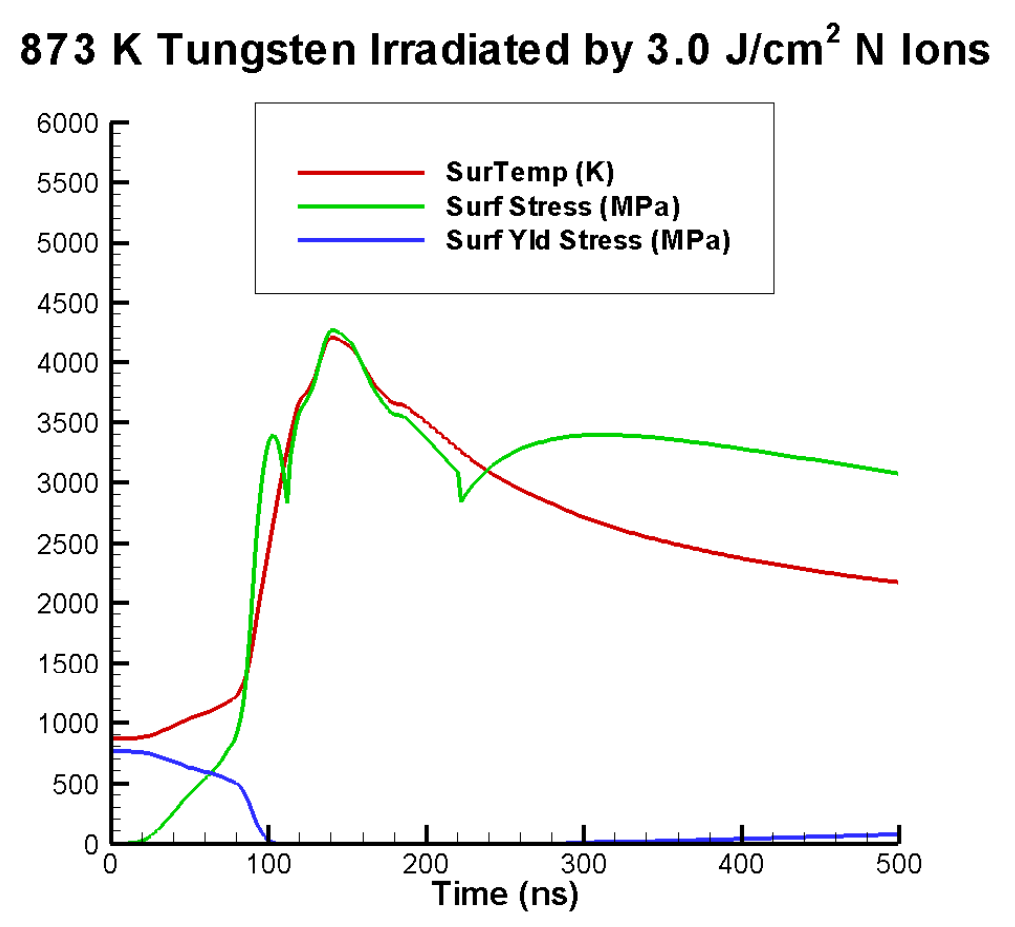
Peak Surface Temperature is Sensitive to Ion Type

- Predicted RHEPP Peak surface temperatures show change in slope at melting.
- Pre-shot heating of the sample is not just an additive effect because of temperature dependence of properties.
- Higher surface temperatures are seen for N irradiation.

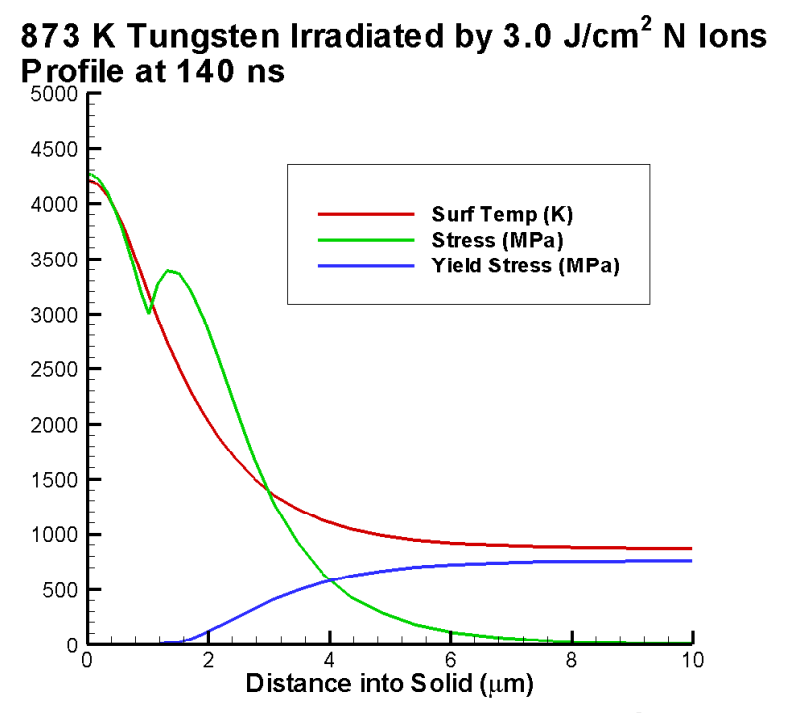


Melted Case Sees Substantial Yielded Material

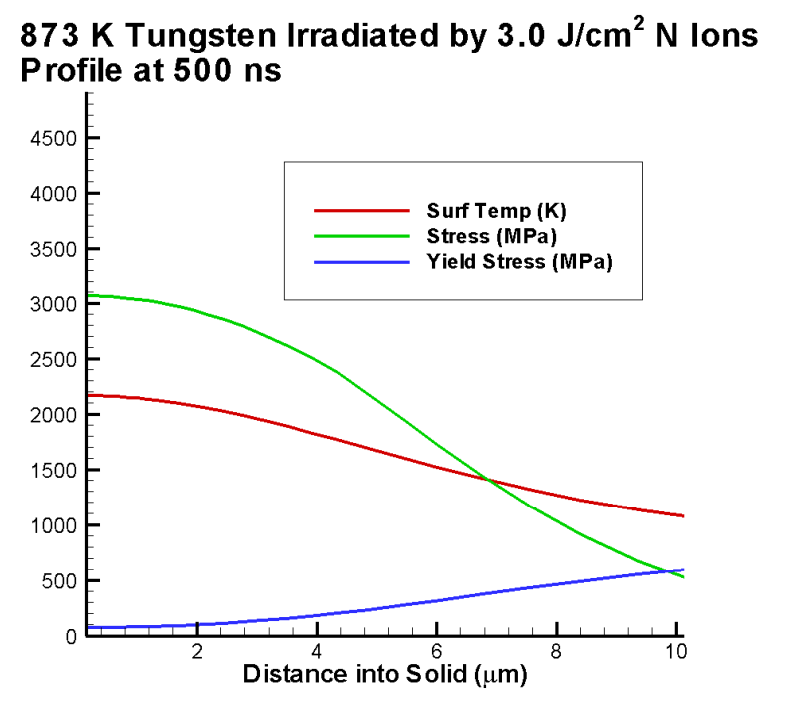
When temperature goes beyond melting, stress model and data is invalid and "stress" values are meaningless.



Yielded region 4 μm thick at 140 ns



Yielded region 10 μm thick at 500 ns



The Mie-Grueneisen EOS Captures Important Solid State Physics

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

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

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

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. $\frac{1}{V_0}, C_v, c_s$

In the Future, We Want to Try the Mie-Grueneisen EOS inside BUCKY to Model RHEPP and Z Experiments

1. M-G EOS in BUCKY will predict plastic flow with thermal and shock effects.
2. High strain rate and grain effects are probably playing some role in the roughening (grain size effect seen experimentally on RHEPP).
3. M-G EOS could be adapted to include grain and strain rate effects on yield stress and cohesive energy.
4. Once we are happy with Z and RHEPP modeling, apply M-G EOS to chamber wall simulations.