Plasma Flow in the Laser Target for the CRASH Project: Sensitivity to the Choice of EOS for Non-Ideal Plasmas

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The CRASH project: main objective

- **CRASH stands for Center for RAdiative Shock Hydrodynamics**
- **Five year project, sponsored as the scientific program supported by the National Nuclear Security Administration (part of DOE)**
- **Key objectives:**
    - **Predictive Science**
    - **Uncertainty Quantification**

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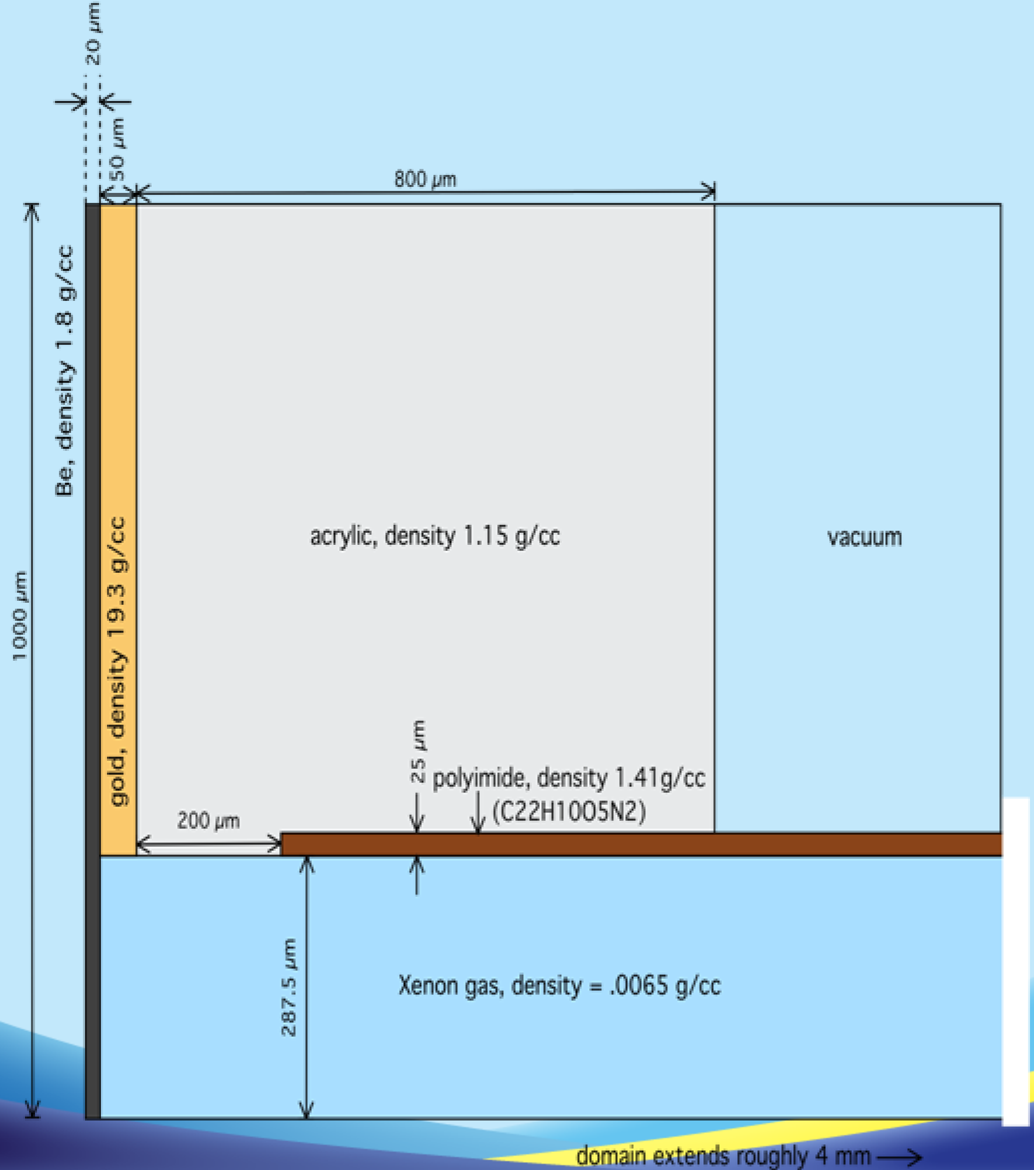
Geometry of a target for OMEGA.



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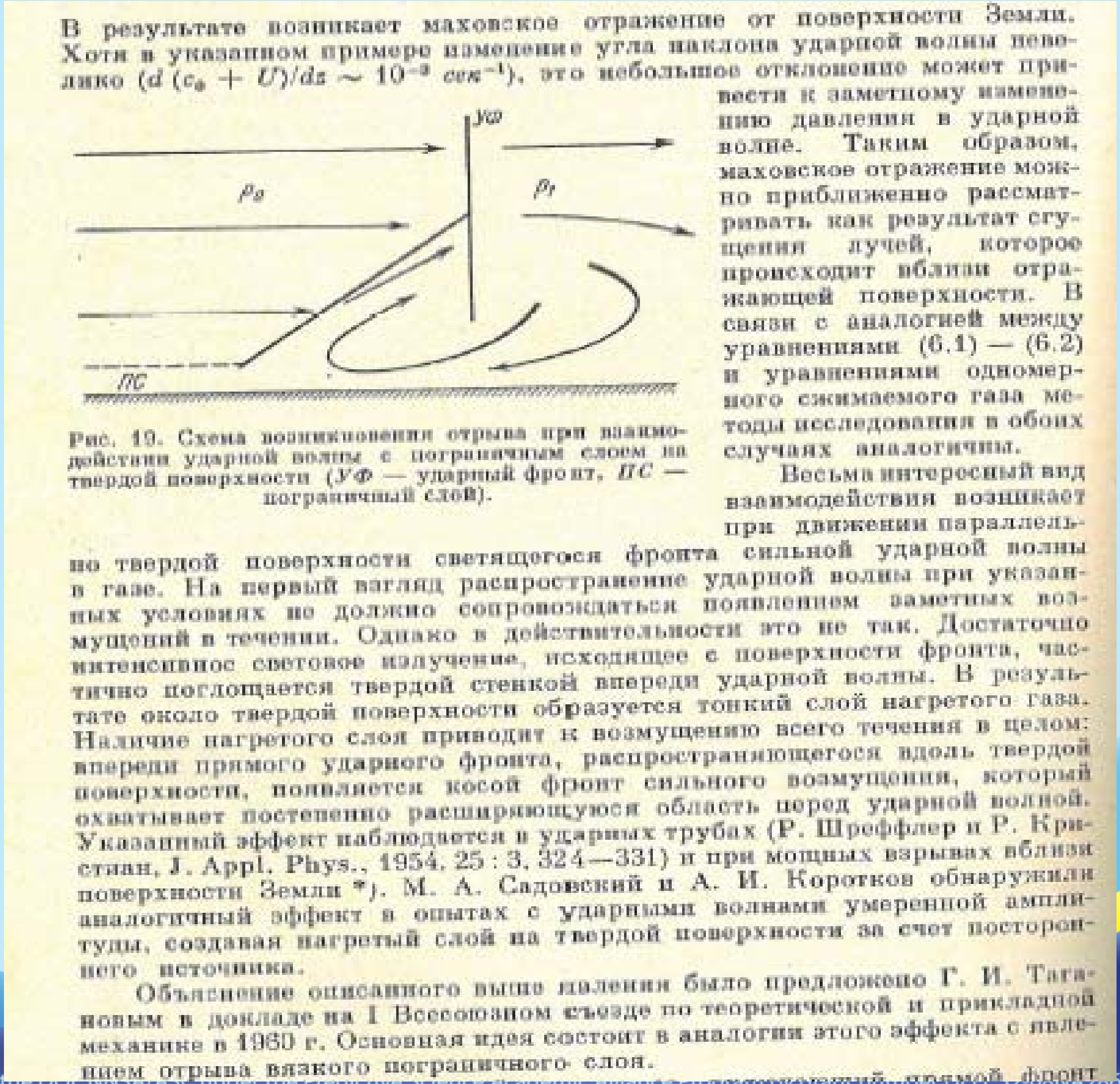
Radiative shock + solid wall what can occur?

- **Page 310 from the book:** Механика в СССР за **50** лет



В результате возникает маховское отражение от поверхности Земли. Хотя в указанном примере изменение угла наклона ударной волны невелико ($d(c_0 + U)/dz \sim 10^{-3}$ $сек^{-1}$), это небольшое отклонение может привести к заметному изменению давления в ударной волне. Таким образом, маховское отражение можно приближенно рассматривать как результат сгущения лучей, которое происходит вблизи отражающей поверхности. В связи с аналогией между уравнениями (6.1) — (6.2) и уравнениями одномерного сжимаемого газа методы исследования в обоих случаях аналогичны.

Рис. 19. Схема возникновения отрыва при взаимодействии ударной волны с пограничным слоем на твердой поверхности (*УФ* — ударный фронт, *ПС* — пограничный слой).

Весьма интересный вид взаимодействия возникает при движении параллельно твердой поверхности светящегося фронта сильной ударной волны в газе. На первый взгляд распространение ударной волны при указанных условиях не должно сопровождаться появлением заметных возмущений в течении. Однако в действительности это не так. Достаточно интенсивное световое излучение, исходящее с поверхности фронта, частично поглощается твердой стенкой впереди ударной волны. В результате около твердой поверхности образуется тонкий слой нагретого газа. Наличие нагретого слоя приводит к возмущению всего течения в целом: впереди прямого ударного фронта, распространяющегося вдоль твердой поверхности, появляется косой фронт сильного возмущения, который охватывает постепенно расширяющуюся область перед ударной волной. Указанный эффект наблюдается в ударных трубах (Р. Шреффлер и Р. Кристиан, J. Appl. Phys., 1954, 25 : 3, 324—331) и при мощных взрывах вблизи поверхности Земли *). М. А. Садовский и А. И. Коротков обнаружили аналогичный эффект в опытах с ударными волнами умеренной амплитуды, создавая нагретый слой на твердой поверхности за счет постороннего источника.

Объяснение описанного выше явления было предложено Г. И. Тагановым в докладе на I Всесоюзном съезде по теоретической и прикладной механике в 1960 г. Основная идея состоит в аналогии этого эффекта с явлением отрыва вязкого пограничного слоя.

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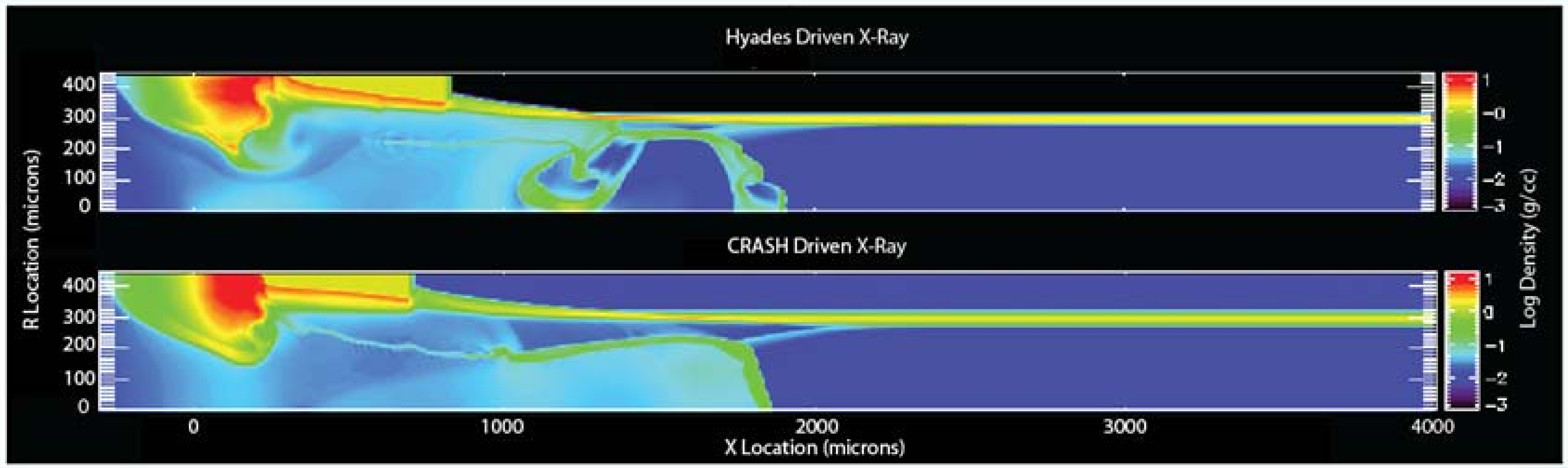
On axis feature (is often observed in simulations, never in the experiment)



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On-axis feature: Mach reflection of the axially symmetric convergent shock wave

- *In the cylindrical tube the "wall shock" forms which is a particular case of axially-symmetric convergent shock waves:*

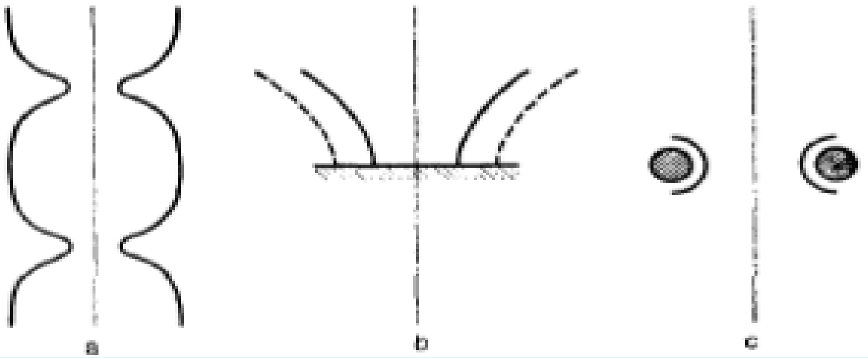

FIG. 4. Axially symmetric, noncylindrical convergent shock waves. a—Cylindrical front with sausage-type perturbations. b—Shock wave in a plasma focus. c—Annular (toroidal) shock wave.

After reflection on the axis the Mach shock forms (usually small)

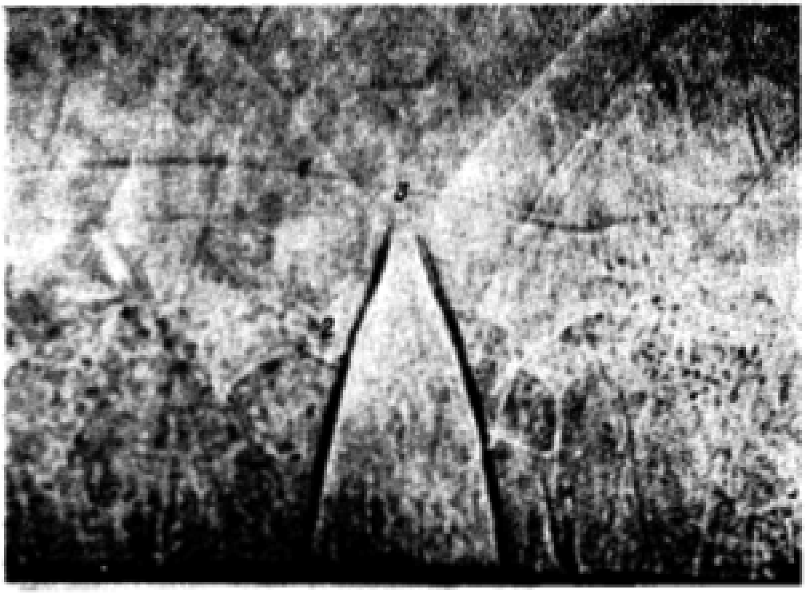

FIG. 6. Appearance of a Mach configuration in the reflection of an annular shock wave from the axis: shadow photography in a direction perpendicular to the axis. *1*—converging front of the shock wave; *2*—reflected wave; *3*—high-velocity jet of gas propagating along the axis.

Hydrodynamic cumulative processes in plasma physics

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Usp. Fiz. Nauk **160**, 143–166 (November 1990)

On-axis feature is the must, why don't we observe it?

- The universal character of the Mach reflection for the axially symmetric convergent waves had been proved theoretically (the Witham method), experimentally (toroidal discharge) and numerically (in 1987-1991, MacCormack and Lax-Wendroff schemes with the conservative smoothing).

- In the CRASH geometry the Mach shock should first form behind the main shock wave front and then pass the main shock wave forming the jet precursor (as we see in simulations)

- Theoretically, the "on-axis feature" formation is the must – why don't we see it in the experiment?
    - The size of the Mach shock is usually small, especially for weak convergent shocks
    - The convergent wall shock is probably too strong in the simulations and weaker in reality (wrong Xe opacity? Polyimide EOS?)
    - The feature may be smeared out by ion viscosity or turbulent mixturing in shocked Xe.

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Our EOS and opacity functions support our UQ effort

- Outline
  - Why do we need EOS functions and opacities?
  - Why do we need the built-in model for them (not tables?)
  - Scheme of calculation:

    - Pressure, internal energy density, specific heat and other thermodynamic derivatives.

    - Planck and Rosseland multi-group opacities.
  - Helmholtz free energy (statistical sum method).
  - Cross-model comparison

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Why do we need the EOS and opacity DATA?

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0,$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot \left[\rho \mathbf{u} \otimes \mathbf{u} + (P + P_{rad})I\right] = 0,$$

$$\frac{\partial (\rho \frac{u^2}{2} + E)}{\partial t} + \nabla \cdot \left[\mathbf{u}(\rho \frac{u^2}{2} + E + P + P_{rad})\right] = P_{rad} \nabla \cdot \mathbf{u},$$

$$\frac{\partial E_g}{\partial t} + \nabla \cdot (\mathbf{u} E_g) - \frac{1}{3} \nabla \cdot \mathbf{u} \int_{\varepsilon_g} \frac{\partial (\varepsilon E_g)}{\partial \varepsilon} d\varepsilon = -\frac{1}{3} E_g \nabla \cdot \mathbf{u} +$$

$$+\nabla \cdot \left(\frac{cC_g(T_g)}{3\kappa_{Ross}} \nabla T_g\right) + c\kappa_{Planck} C_g(T)(T - T_g)$$

$$P = P_{EOS}(E,\rho), \quad T = T_{EOS}(E,\rho),$$

$$T_g(E_g): \quad E_g = \int_{\varepsilon_g} B(T_g)\, d\varepsilon, \quad P_{rad} = \frac{1}{3} \sum_g E_g,$$

$$C_g(T) = \int_{\varepsilon_g} \frac{dB(T)}{dT} d\varepsilon, \quad E_g = \int_{\varepsilon_g} E_\varepsilon\, d\varepsilon$$

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What do we need?

- Relationships between
  - - mass density,
  - - pressure,
  - - electron pressure,
  - - internal energy density,
  - - electron temperature.

  For xenon, beryllium and plastic!

- For high-resolution schemes we need the sound speed, that is:

$$C_s = \sqrt{\left(\frac{\partial P}{\partial \rho}\right)_S} = \sqrt{\frac{\gamma P}{\rho}}, \quad \gamma = \frac{\rho}{P}\left(\frac{\partial P}{\partial \rho}\right)_T + \frac{T}{C_V P}\left(\frac{\partial P}{\partial T}\right)_\rho^2$$

- Therefore we also need:
  - - all thermodynamic derivatives…
  - - …along the ionization equilibrium curve.

- We need multi-group opacities now and frequency-dependent opacities in the future.

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There are tables, why do we develop models?

- First, it is interesting and attractive for all the involved sides.

- For the uncertainty quantification: we use the model, based on:
  - first principles;
  - specified assumptions (LTE);
  - controllable list of the input parameters
    - ionization potentials;
    - excitation energies, multiplicities;
    - cross-sections;
    - oscillator strengths etc.

- Consistency: calculate opacities and EOS under the same assumptions.

- We benefit from a capability to verify our models with the “gold standard” models (such as SESAME). However, the use of black-box models sometimes appears problematic.

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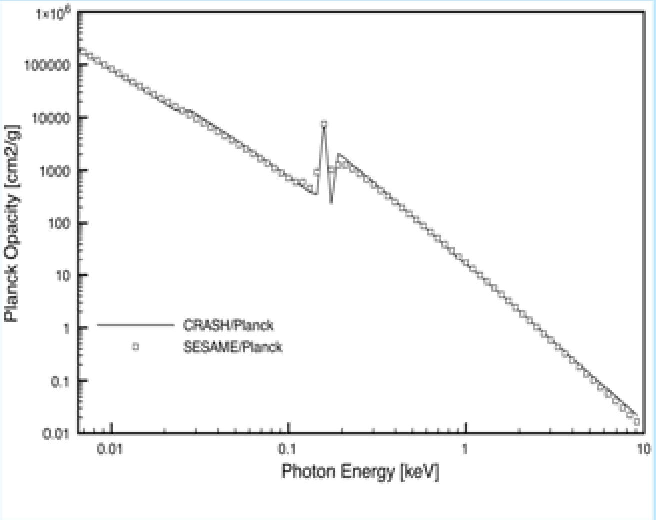
Why not use black-box external model?



- Similarity and good overall agreement of the “black-box” model with the “transparent” model.
- The partition functions in SESAME differ from those we use for EOS in CRASH, raising the issues of:
  - consistency of EOS and opacity models;
  - utility of uncertainty quantification.

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“Trivially-correct” computational model

- The Helmholtz free energy includes the contributions from
  - -Fermi statistics in the free electron gas;
  - -Coulomb interactions (the Madelung energy);
  - -Excited levels;
  - -Pressure ionization (eliminate weakly-bound states)

- Minimizing the Helmholtz free energy yields:

$$\frac{\partial F}{\partial N_{i+1}} + \frac{\partial F}{\partial N_e} - \frac{\partial F}{\partial N_i} = 0$$

- The ionization equilibrium includes the following effects:
  - -The ‘continuum lowering’ affects not only the absorption spectrum, but also thermodynamics (via ionization).
  - - The Fermi statistics effect, ‘the exchange interaction’, affects the pressure both directly and via the ionization.

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Thermodynamic consistency

- We may both use the inline EOS and use it to fill in tables
- The internal energy density and pressure are expressed in terms of the derivatives of the Helmholtz free energy:

$$\mathcal{E} = -\frac{T^2}{V}\left(\frac{\partial}{\partial T}\left(\frac{F}{T}\right)\right) = \mathcal{E}_i + \mathcal{E}_e, \qquad \mathcal{E}_i = \frac{3}{2}Tn_a, \qquad \mathcal{E}_e = n_a\left[\frac{3}{2}TZR^{+} + \langle E_i^{*}\rangle\right],$$

$$P = -\frac{\partial F}{\partial V} = P_i + P_e, \quad P_i = n_a T, \quad P_e = n_a\left[TZR^{+} - V\langle\frac{\partial E_i^{*}}{\partial V}\rangle\right],$$

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More models

- EOS for polyimide (Konstantin V. Khischenko, JIHT)
- Opacities for polyimide (Marcel Klapisch, ARTEP)
- NonLTE effects (Michel Busquet, ARTEP)
- Xenon multigroup opacities – uncertainty if also very high.

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Validation and Verification: cross-model comparison

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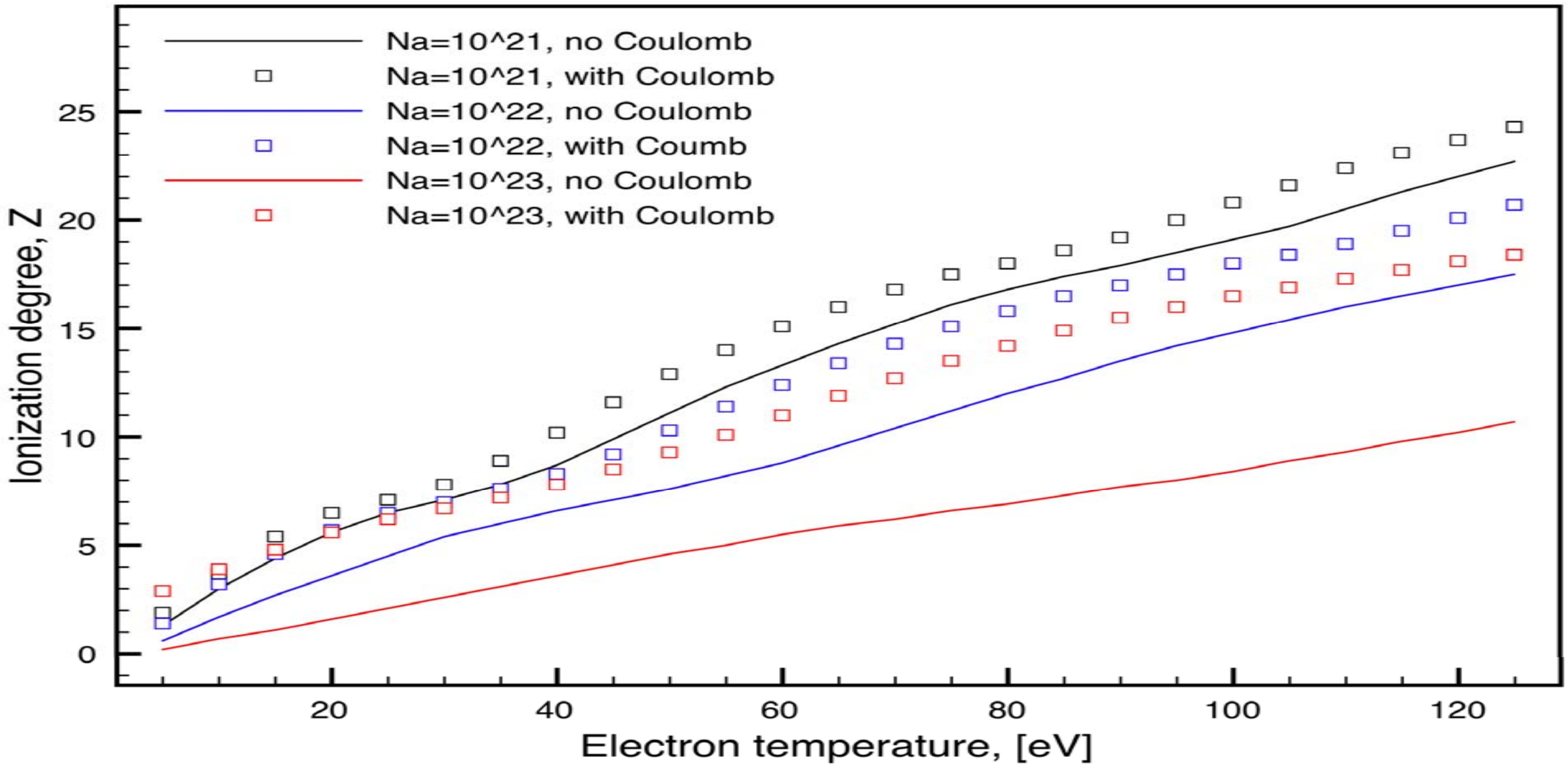
Testing EOS

- Comparison with Hyades and SESAME models for EOS: the deviation in the calculated ionization degree is ~0.2.
- Should compare the partition functions, rather than the averages. More challenging is the comparison of opacities.



Validation and Verification: Include the Non-LTE effects

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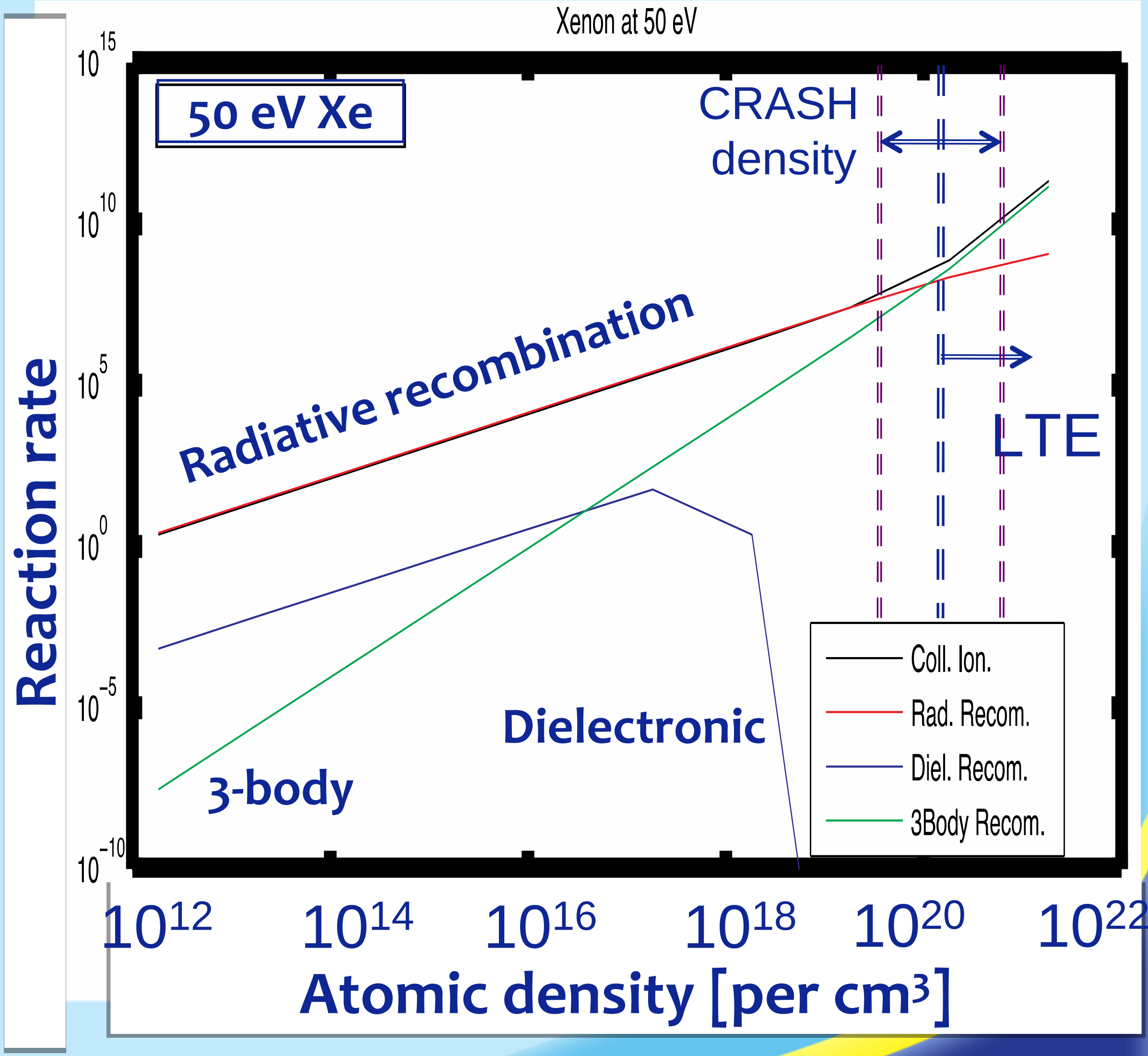
Reaction rates in xenon are a possible issue for CRASH

- **LTE happens when**
  - o **radiative recombination (red curve) << 3-body collisional recombination (green curve)**
  - o **Then collisions ensure that Z=Z(Te) only.**

- **Non-LTE happens when**
  - o **radiation recombination dominates over 3-body recombination**
  - o **The coronal model then applies: one-source-two-sinks of free electrons, which affect the ionization degree.**
  - o **For optically thin media, of course**

- **Prof. G.A.Moses raised this issue**



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NonLTE may impact the CRASH problem

- energy balance :

  for same Etot, more in electron kinetic energy, and less in ionization "internal" energy

- thermal conduction :

  as average charge is lower,

  electron conduction (and laser absorption) is reduced

- radiative energy :
  - less coupling of radiation with matter
  - X-ray conversion of E_{laser} reduced
  - x-ray precursor (of shock wave, ...) has larger extent

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Principle of the RADIOM model

- Non-LTE of charge state distribution (and excited states to some extent) is mimicked by an "ionization temperature" T_z
- We are able to derive numerically T_z from N_e, T_e, {hnu,Erad/Brad}
- Non-LTE total energy is a function of Eint(T_z), Zbar(T_z), T_e (and r_o) :

$$E_{tot}^{NLTE} - \frac{3}{2} k_B \rho Z^* (T_z) \times (T_e - T_z) = E^{LTE} (T_z)$$

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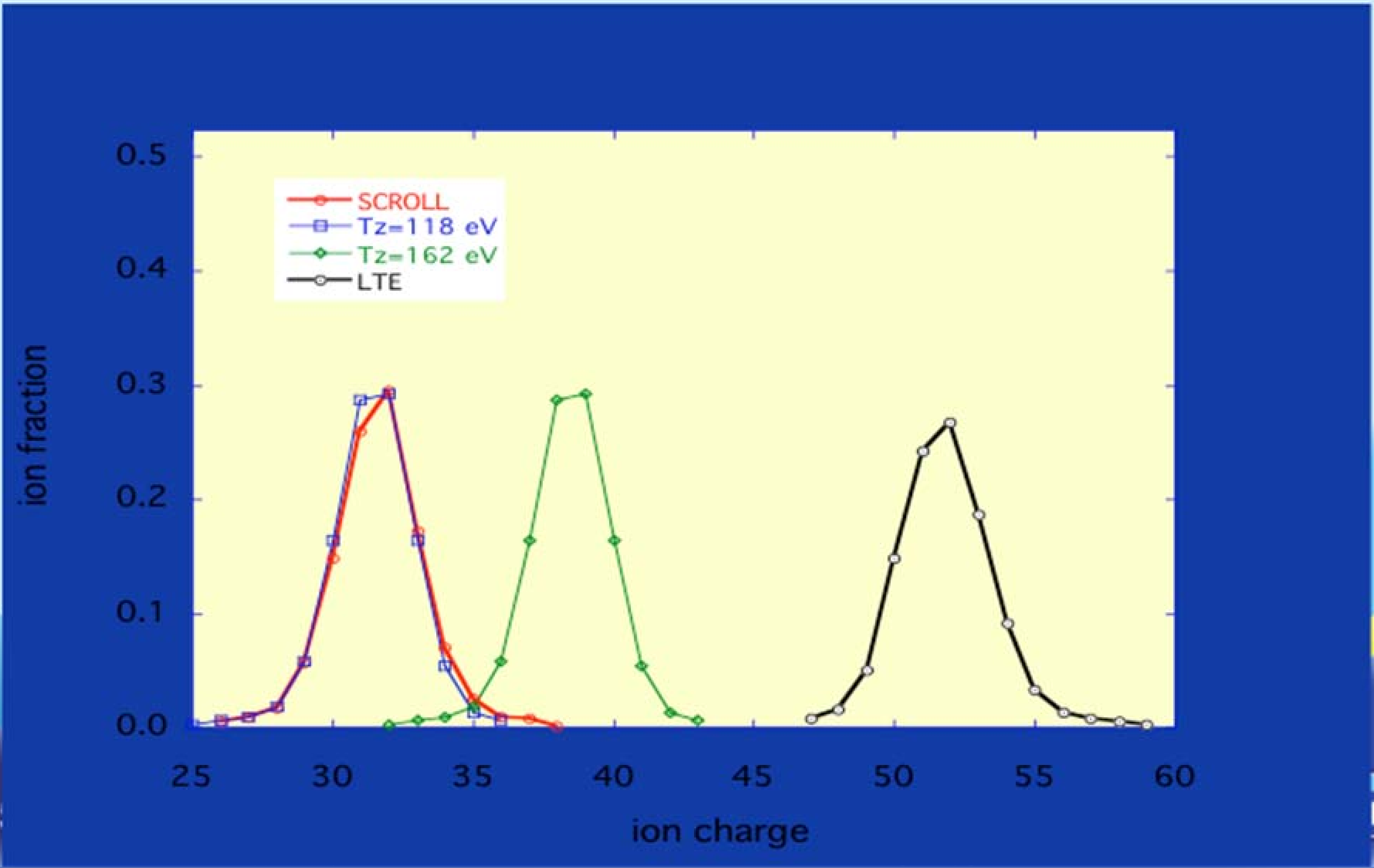
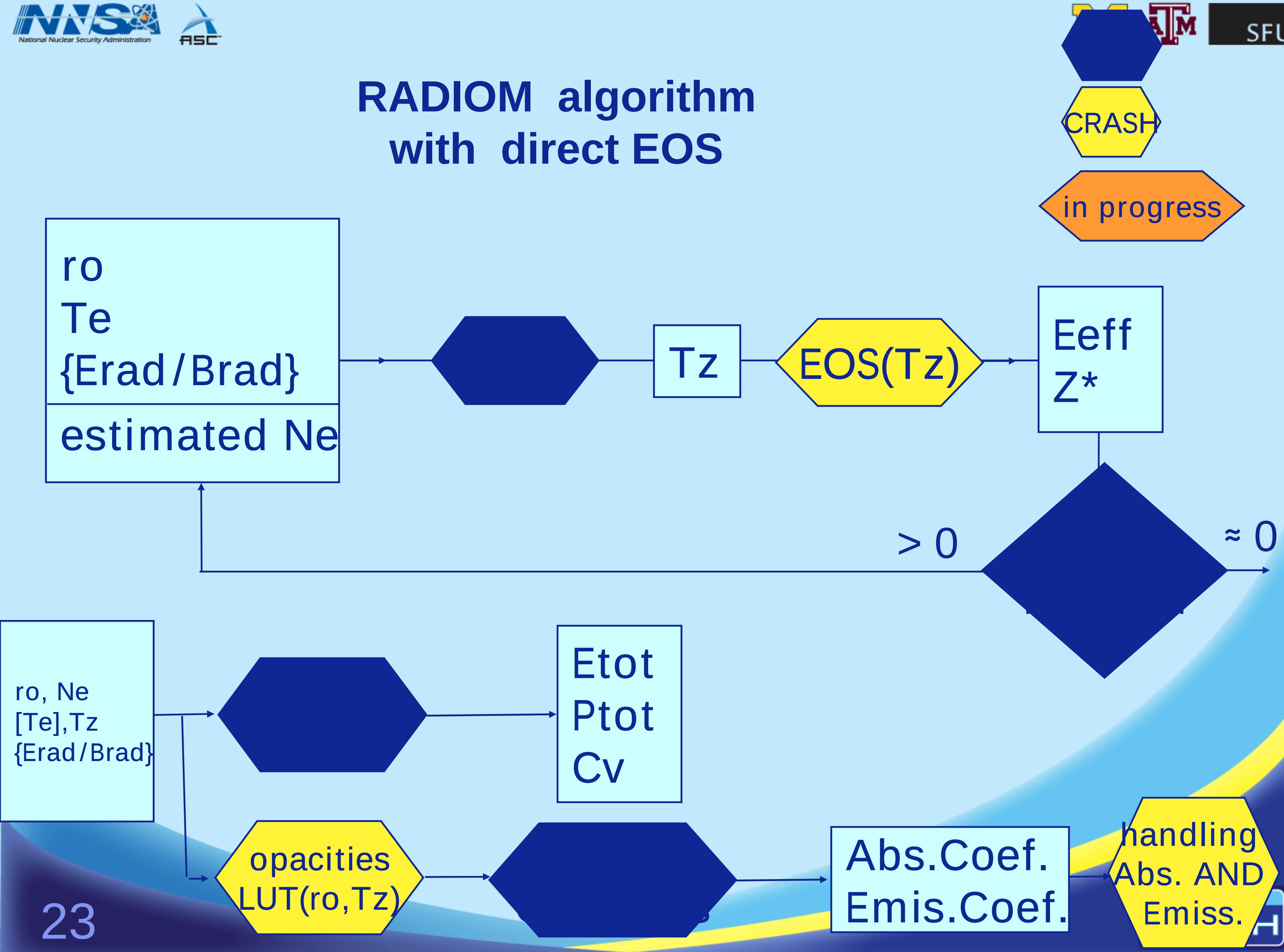
RADIOM reduces the effective ionization in a manner consistent with the SCROLL model



RADIOM algorithm with direct EOS



CRASH

in progress

ro
Te
{Erad/Brad}

estimated Ne

Tz

EOS(Tz)

Eeff
Z*

> 0

≈ 0

ro, Ne
[Te],Tz
{Erad/Brad}

Etot
Ptot
Cv

opacities
LUT(ro,Tz)

Abs.Coef.
Emis.Coef.

handling
Abs. AND
Emiss.

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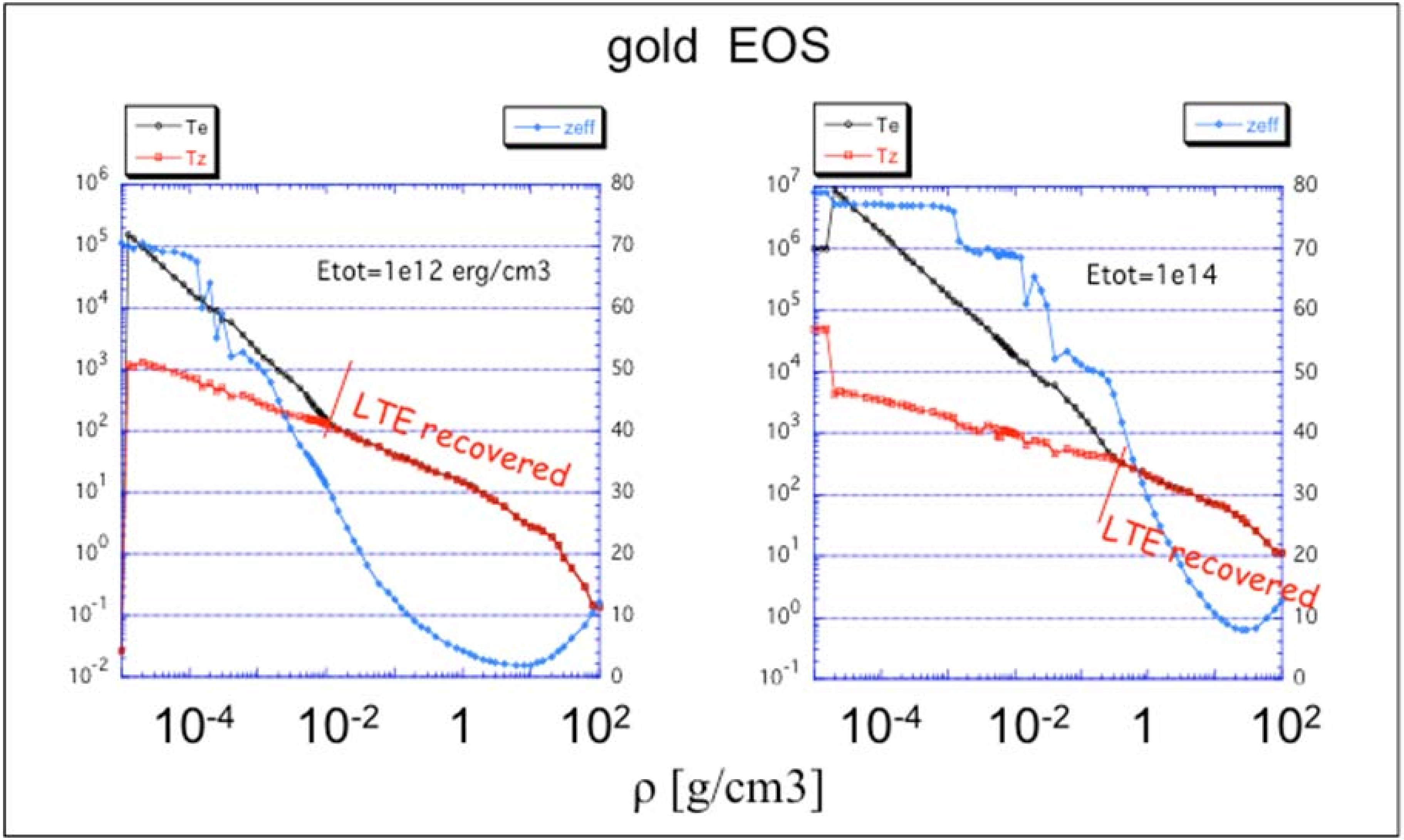
Test result: inverse EOS for gold



The coronal model is not enough for CRASH

- In the (solar) corona the “back-lighter” (the photosphere) has a radiation temperature much LOWER than T_e in the corona (half eV vs hundreds eV). Contrary to our case.
- We may need more electrons, while the coronal model gives us less electrons.
- Need to implement the RADIOM/CRASH coupling for the out-of-equilibrium HOT radiation (hundreds eV vs tens eV).
- This is now in progress.

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