Development of a Transport and Microphysics Capability for Simulations of Shock-Produced Plasmas using Hytrac

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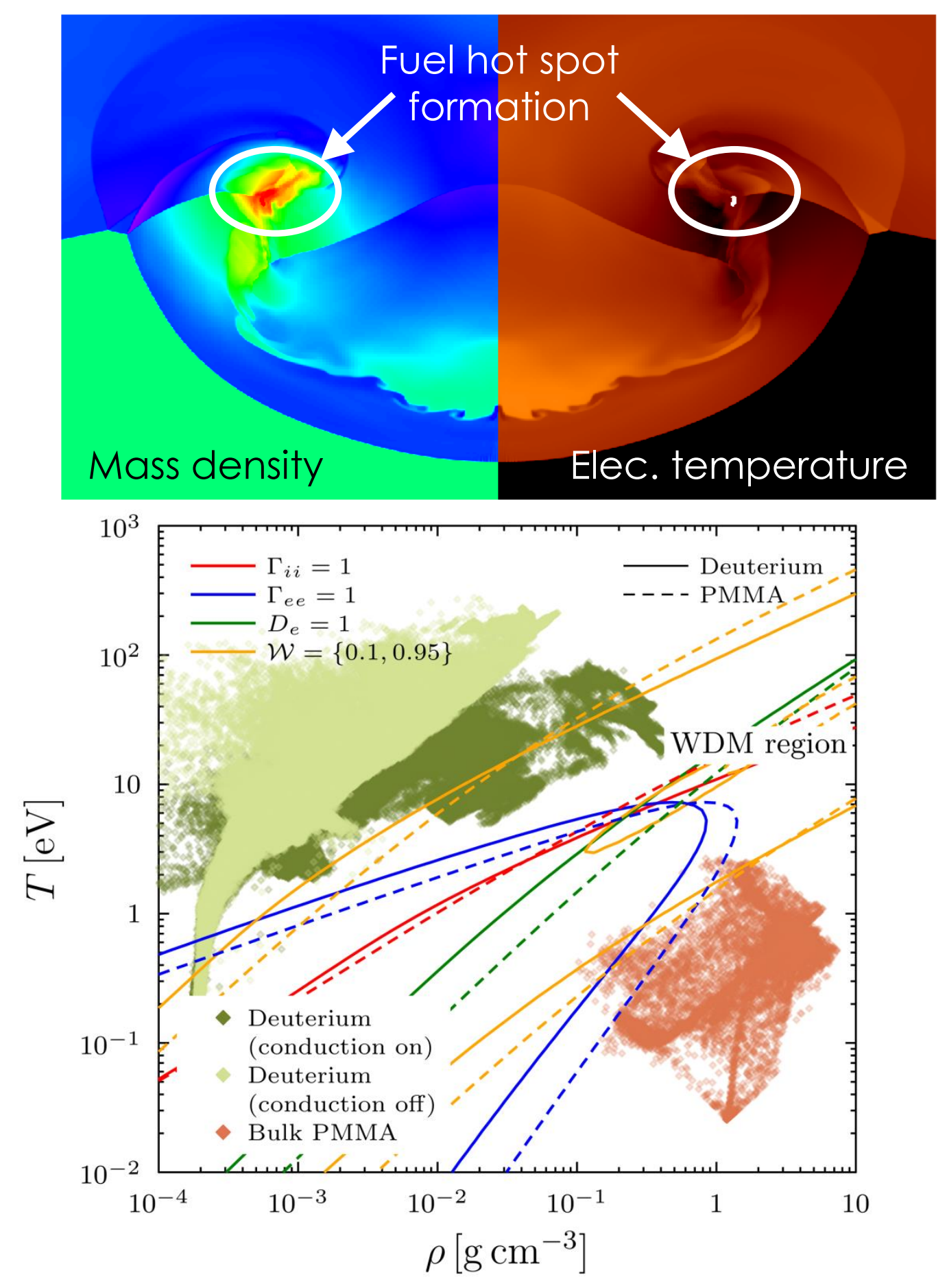
Motivation

- First Light Fusion (FLF) is researching ICF with novel target designs utilising strong shocks driven by hyper-velocity projectiles and EM launch systems.
- Proprietary target designs are being developed and understood using our in-house front tracking hydrodynamics code Hytrac.
- Experiments designed to deliver proof-of-concept and numerical benchmarking data focus on the well-known asymmetric cavity collapse case (Fig. 1 upper panel), which is challenging to model and produces plasmas with conditions relevant to the warm dense matter (WDM) regime (Fig. 1 lower panel).
- Hytrac is being developed from the ground up to deliver a robust multi-physics capability, of which equation of state (EoS), transport, microphysics and radiative effects form core components.


Fuel hot spot formation

Mass density

Elec. temperature

Fig. 1: Hytrac simulation of asymmetric cavity collapse induced by an aluminium projectile moving at 30 km/s (top). Thermal conduction has a significant effect on the evolution of the deuterium in the cavity (bottom).

Ionisation model

- All transport and microphysics models for plasmas rely on input from an ionisation model.
- Simple approaches such as the Thomas-Fermi model fail to capture atomic structure.
- Important around solid densities for temperatures similar to shell ionisation energies.
- We use the SpK model, which uses Busquet's approach [1] with a degeneracy-corrected Saha-Boltzmann solver to deliver LTE and nLTE population kinetics.
- The excitation energies of all configurations is supplemented with NIST data.

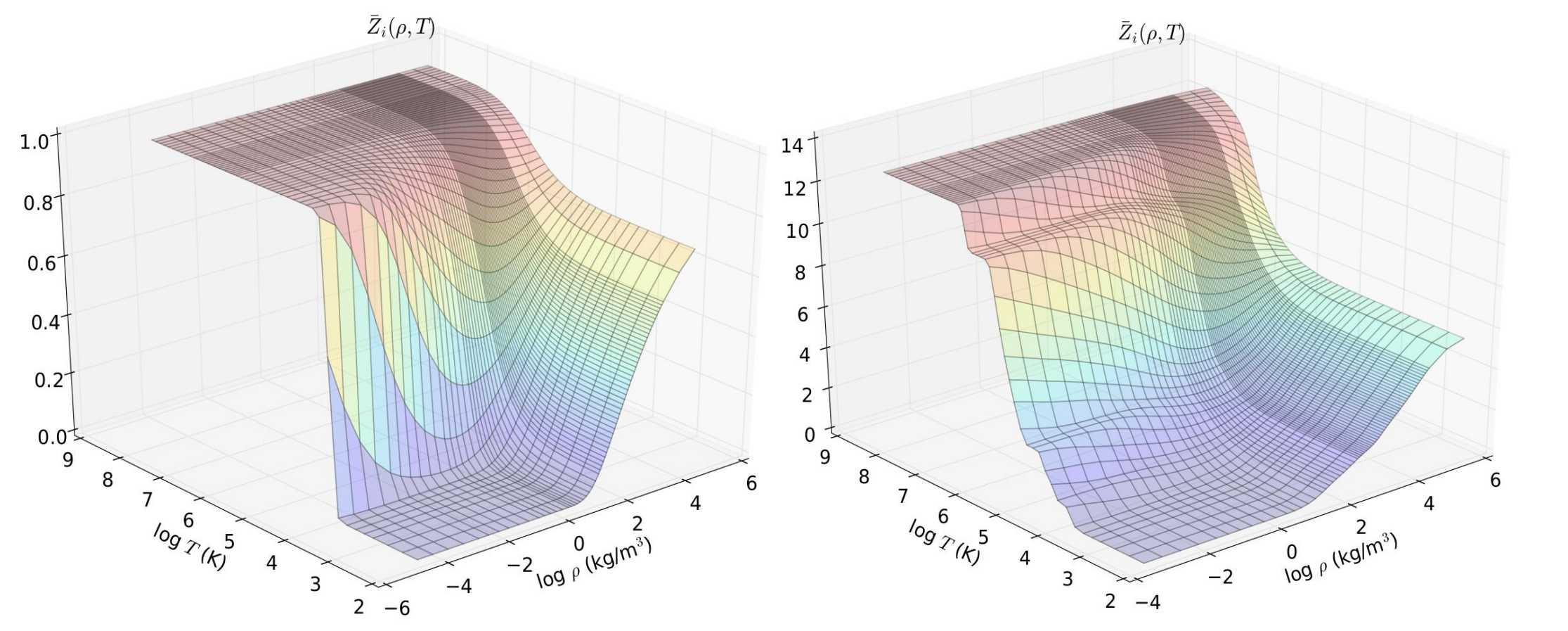


Fig. 2: Surface plots on the density-temperature plane of the mean ionisation state predicted by the SpK model for deuterium (left) and aluminium (right). The ionisation for STP conditions is determined by data; e.g. measured Fermi energy.

Electron thermal conductivity model

- Electron conductivities are required for many materials over a large ρ-T_e-T_i space.
- A flexible and numerically inexpensive approach is the Lee-More model [2,3].
- Significant modifications can be made to improve accuracy around solid phase [4].
- Electrical resistivity (for use in MHD) and ion thermal conductivity use a similar formalism; these are not presently important for our benchmarking and validation experiments.

- Use RTA formalism [2]:

$$\kappa_e = \frac{n_e v_e^2 k_{\mathrm{B}}}{\omega_{\mathrm{pe}}} \left[I_2(\eta) - \frac{I_1^2(\eta)}{I_0(\eta)} \right] R_e$$

$$I_n(\eta) = \frac{4}{3\sqrt{\pi}} \int_0^\infty \mathrm{d}x\, x^{n+\frac{3}{2}}\, y(x) \times F_{-1}(\eta - x)/F_{1/2}(\eta)$$

- The dimensionless collision frequency is:

$$y(x) = \omega_{\mathrm{pe}} \left[\frac{1}{\nu_{e-i}(x) + \nu_{e-n}(x)} + \frac{1}{\nu_{e-i}^{\mathrm{WDM}}} + \frac{k_s}{\nu_{e-ph}} \right]$$

- Ansatz form of the e-e correction [5]:

$$R_e(\eta) = \frac{R_e^{-\infty}}{1 + e^{\eta - \eta_0}} + \frac{1}{1 + e^{\eta_0 - \eta}}$$

$$R_e^{-\infty} \approx \frac{5}{2} \frac{c_0 + c_1 \bar{Z}_i}{1 + c_2 \bar{Z}_i}; \; \bar{Z}_i = \frac{\sum_\alpha n_\alpha Z_\alpha}{\sum_\alpha n_\alpha}$$

- Use Rutherford cross section with fitted lnΛ for e-i and Desjarlais fit [3] for e-n scattering.
- For WDM conditions we modify the standard Lee-More ansatz [2]:

$$\nu_{e-i}^{\mathrm{WDM}} \approx \frac{v_e G_1(\eta)}{\sqrt{\pi/2}} \left(\frac{4\pi \sum_\alpha n_\alpha}{3} \right)^{1/3}$$

- For metallic elements we also include a phonon scattering term [4]:

$$\nu_{e-ph} \approx \frac{e^2 k_{\mathrm{C}} \omega_{pi}}{\hbar v_{\mathrm{F}}} \frac{2\beta}{x^2[1 + (x\gamma)^2]^{1/2}}$$

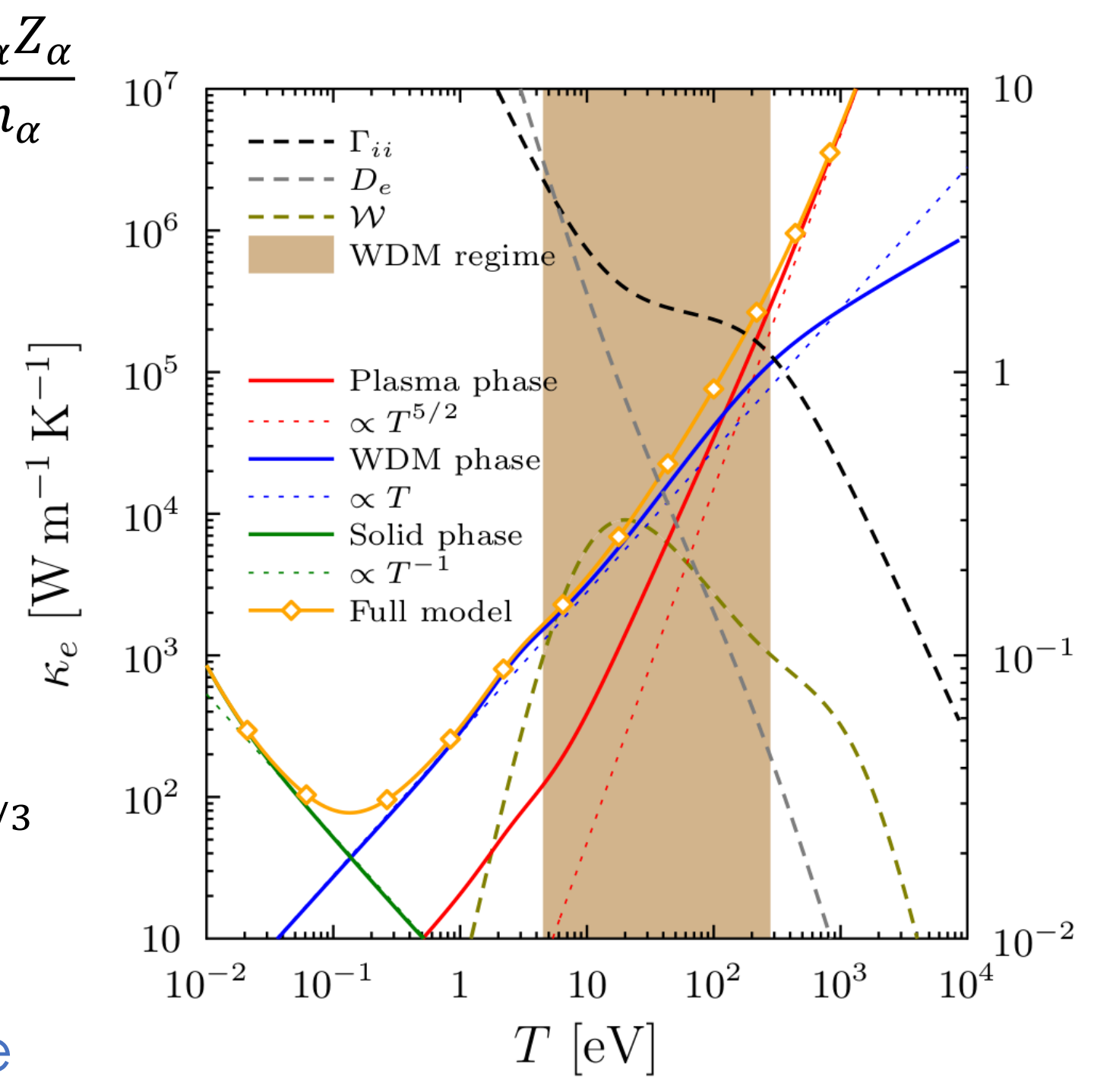


Fig. 3: Plasma model components of the thermal conductivity of solid aluminium (above). The ideal temperature scaling of each part are shown by colour-coded dashed lines.

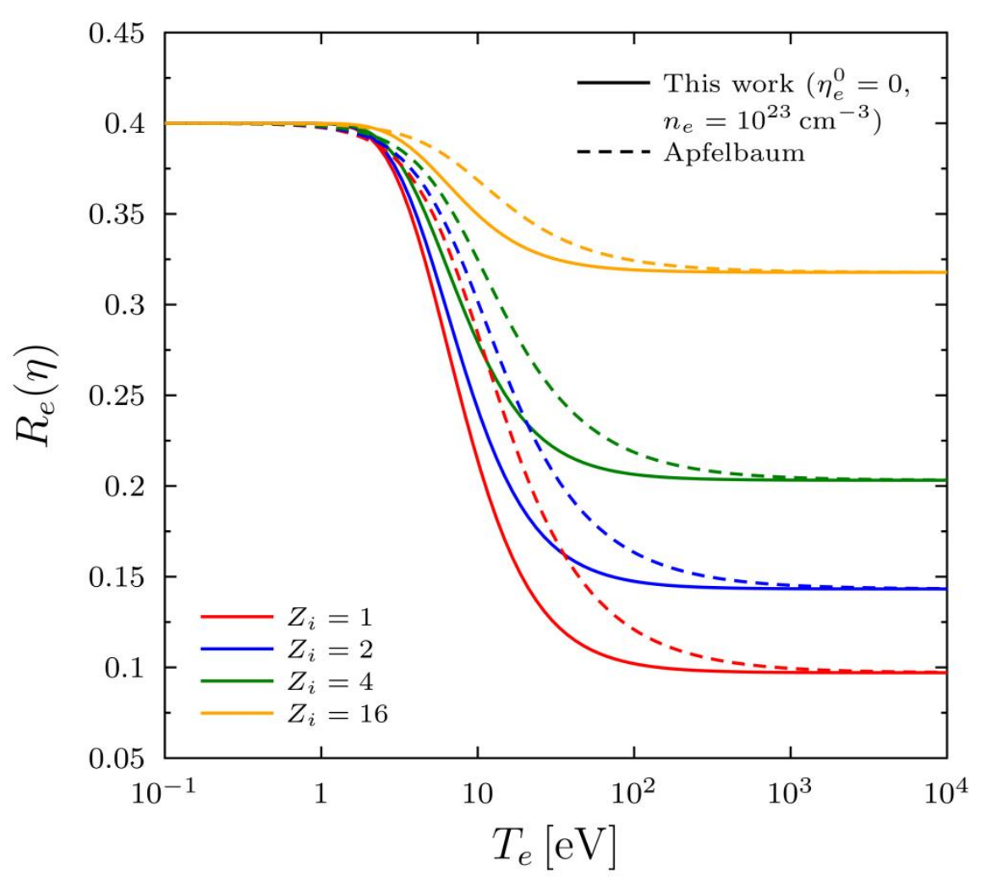
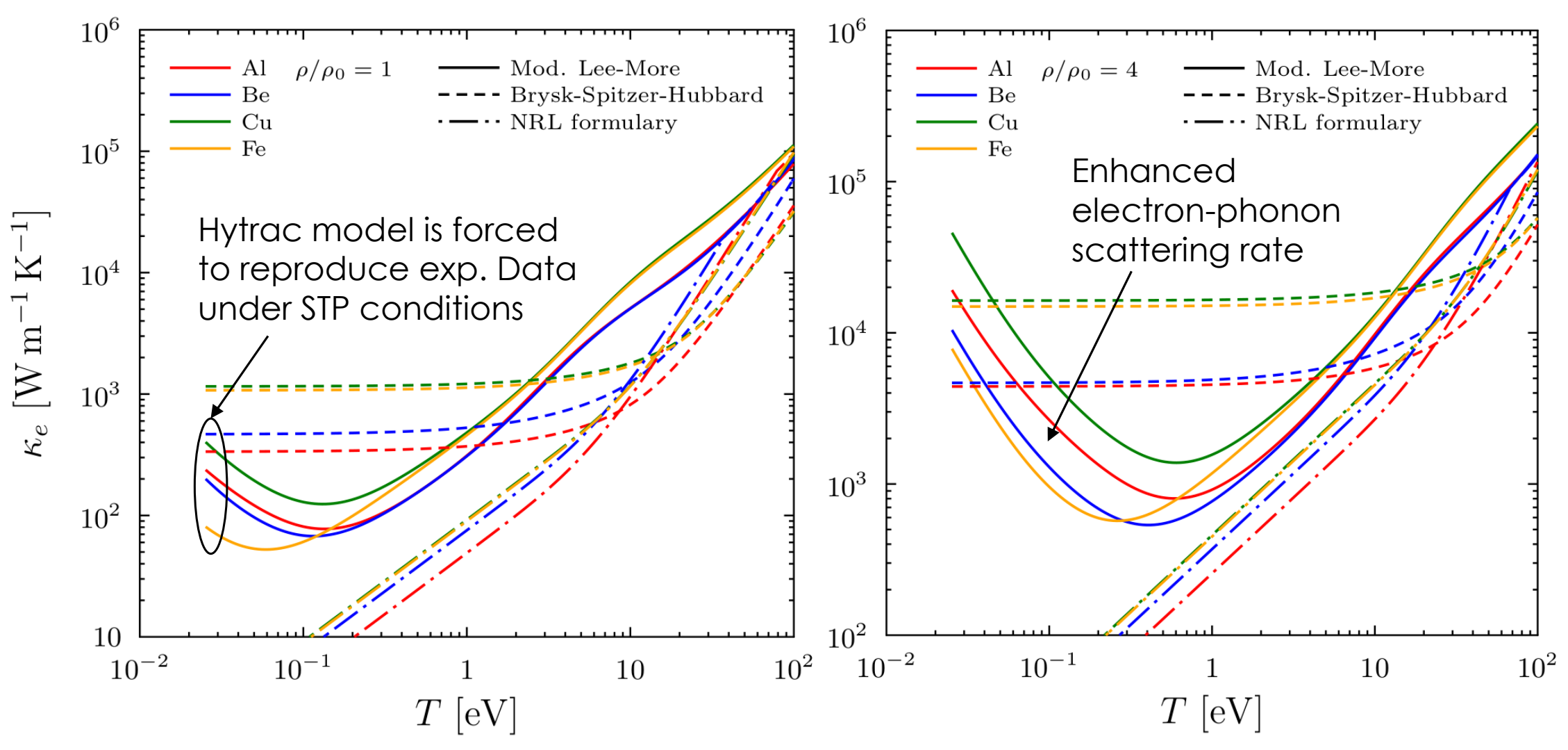


Fig. 4: Behaviour of the electron-electron correction to the (Lorentz) plasma part of the present model.



Hytrac model is forced to reproduce exp. Data under STP conditions

Enhanced electron-phonon scattering rate

Fig. 5: Electron conductivities for Al, Be, Cu & Fe at solid density (left) and 4x compressed (right). The present (solid), Brysk-Spitzer-Hubbard (dashed) and NRL formulary (dot-dashed) models are compared.

Electron-ion relaxation model

- Shock-heated materials involve the production of two-temperature states.
- Affects energetics and feeds back into heat transport and hydro evolution.
- Ions hotter than electrons, such that mode coupling [6] can be neglected.
- Use modified (reduced) Fermi golden rule model [7]:

$$Z_{e\alpha} = \frac{\omega_{\mathrm{pe}}^2 \omega_{\mathrm{p}\alpha}^2 L_{e\alpha}}{(2\pi)^{3/2} v_e^3} k_{\mathrm{B}}(T_e - T_\alpha)$$

$$L_{e\alpha} = \int_0^\infty \frac{dx}{x} \frac{G_{-1}(\eta - x^2)}{|\epsilon_{ee}(k_e^{\mathrm{norm}} x, 0)|^2}$$

$$k_e^{\mathrm{norm}} = (8 m_e k_{\mathrm{B}}\, T_e)^{1/2}/\hbar$$

- Strong electron coupling [8]and finite-wavelength screening [9] are included in the dielectric function:

$$\epsilon_{ee}(k, 0) = 1 + [1 - G_{ee}(k)] \zeta_e^2(k)/k^2$$

- Currently developing CMHNC approach for alternative SLFC.

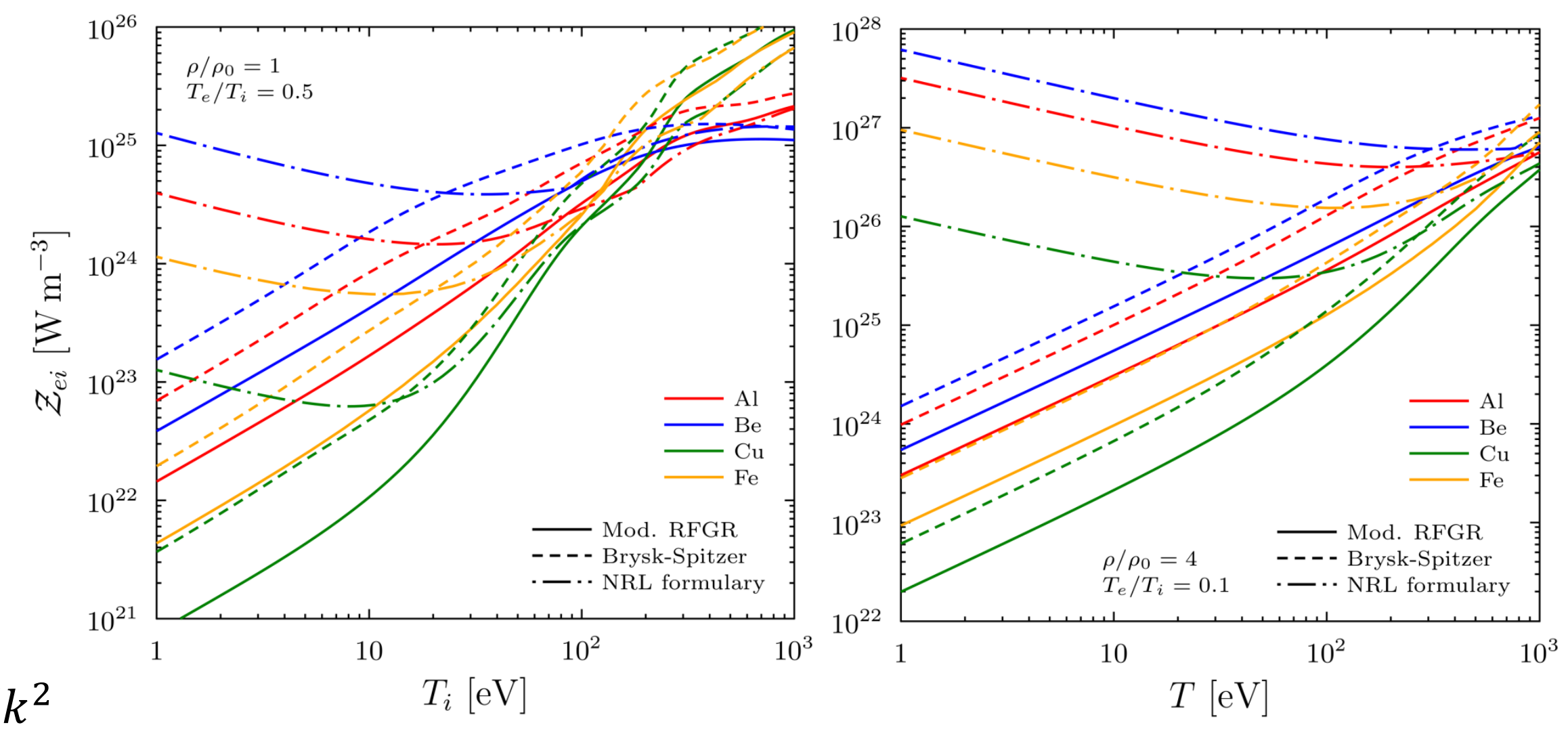
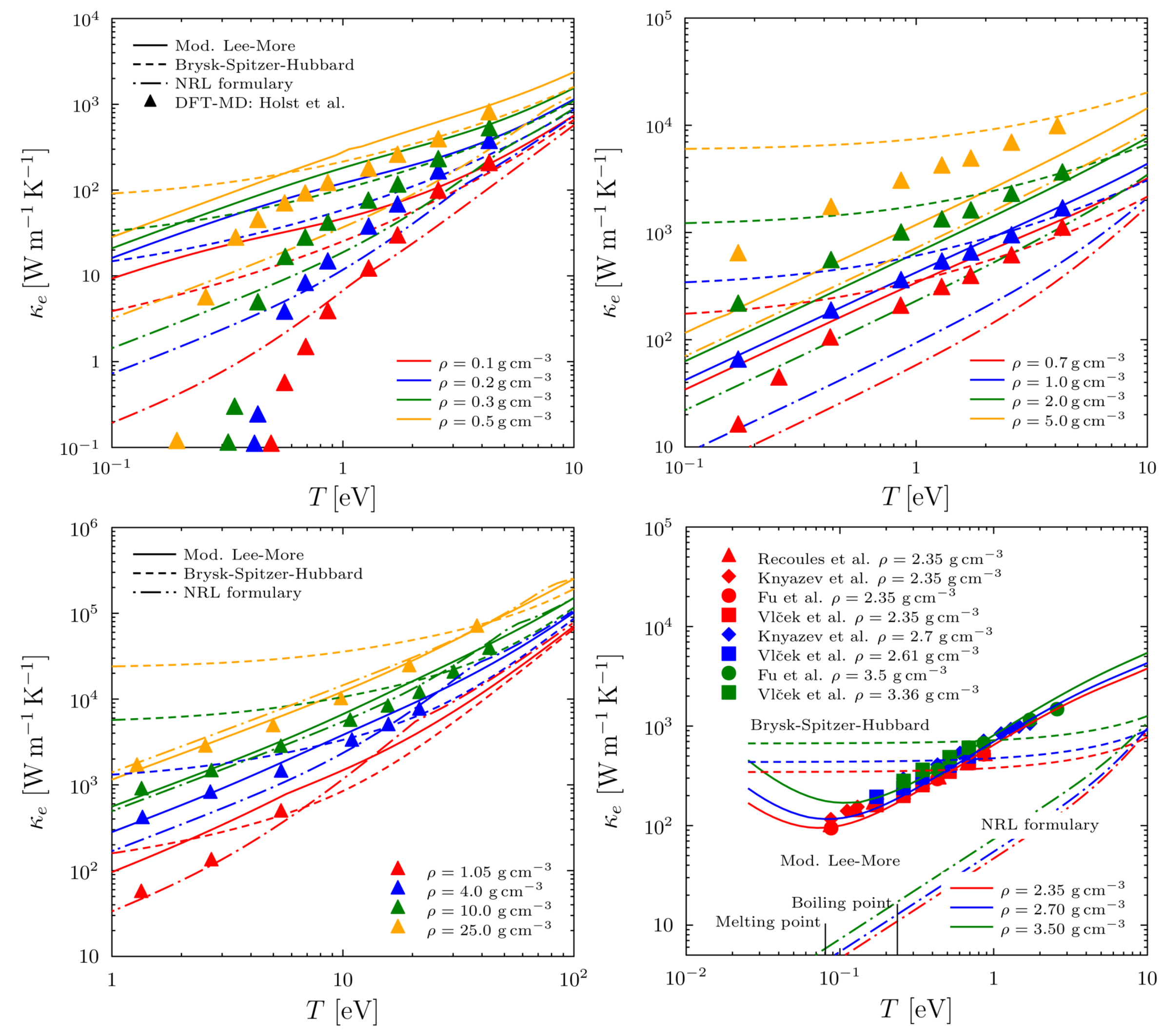


Fig. 6: Electron-ion relaxation rates at constant temperature ratio for solid density (left) and 4x compressed (right) metallic elements. All curves are driven by the SpK ionisation model.

Benchmarking conductivities against DFT-MD



- Comparisons to DFT-MD simulations [10,11] show reasonable agreement for conducting states.
- Insulator-conductor transition in hydrogen is clearly still problematic.
- Demonstrates need for better neutral scattering models.
- Simple metals show very good agreement under WDM conditions.
- An improved treatment for both WDM and neutral scattering contributions are currently being developed.

Fig. 7: Comparison of modified Lee-More approach with DFT-MD data for hydrogen (top panels), CH (bottom left) and aluminium (bottom right).

Comparison of Hytrac and Helios-CR models

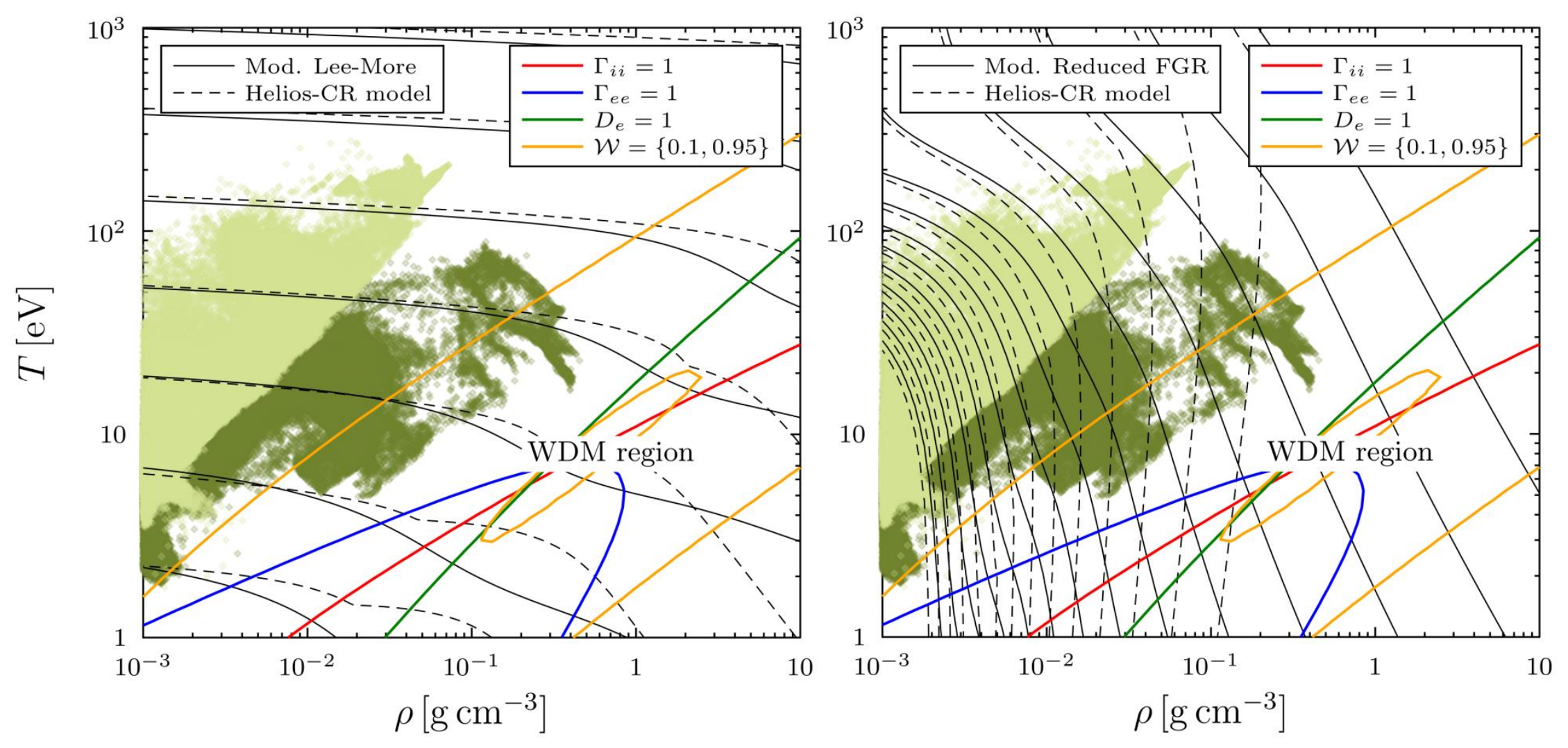


Fig. 8: Contour plots of the electron thermal conductivity (left) and electron-ion equilibration rate with $T_e = 0.5\, T_i$ (right) for deuterium. The present models as used in Hytrac (solid) are compared to those used in the Helios-CR code (dashed).

- Benchmarking of Hytrac against the Helios-CR code [12] in simple geometries is currently being undertaken.
- The models in Helios-CR rapidly break down under conditions relevant to cavity collapse experiments.
- Differences in equilibration rates massive; this may feed back into the thermal conductivity model.
- Differences are even larger for metals, especially in the weakly-ionised regime.

Current and future work

- Extensive sensitivity study of our targets to equation of state and microphysics models.
- Full coupling of the SpK ionisation model output to the thermal conductivity and energy exchange rate models; crucial for multi-component materials, such as plastics.
- More robust treatments for low-temperature effects
  - Electron-neutral and electron-phonon scattering contributions.
- Improved plasma/WDM phase conductivity with Ichimaru-Tanaka-style model [13,14]:
  - Multi-component QHNC model for inter-species correlations
  - Higher-order orthogonal polynomials for better accuracy in ideal plasma regime

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