SIMULATIONS OF ABSORPTION OF FEMTOSECOND LASER PULSES IN COPPER

N.G. Karlykhanov, P.A. Loboda, G.V. Sin’ko,
N.A. Smirnov, A.A. Shadrin

Russian Federal Nuclear Centre – All-Russian Institute of Technical Physics (RFNC-VNIITF)
Snezhinsk, Russia

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Outline

- Simulations of absorption of femtosecond laser pulses in copper using modified ERA hydrocode.
- Thermodynamic functions calculated by using both Full-Potential Linearized Maffin-Tin Orbitals (FP-LMTO) and chemical-picture (CP) model of dense plasma utilizing superconfiguration (SC) approach.
- Comparisons to experimental and other theoretical data.

Modified version of 1D ERA hydrocode

Modeling of femtosecond laser pulse interaction with flat copper targets was done in planar two-temperature approximation with a modified version of 1D Lagrangian ERA(†) hydrocode (laser-pulse absorption, heat conduction, and plasma dynamics).

$$\frac{\partial \varepsilon_e}{\partial t} + P_e \cdot \frac{\partial u}{\partial q} + \frac{\partial W_e}{\partial q} = Q_L - \Delta Q_{ei},$$

$$\frac{d}{dt}\left(\frac{1}{\rho}\right) = \frac{\partial u}{\partial q},$$

$$\frac{\partial \varepsilon_i}{\partial t} + P_i \cdot \frac{\partial u}{\partial q} + \frac{\partial W_i}{\partial q} = \Delta Q_{ei}$$

$$\frac{\partial u}{\partial t} + \frac{\partial P}{\partial q} = 0,$$

$$u = \frac{\partial x}{\partial t},\ dq = \rho \cdot dx,$$

$$P = P_e + P_i$$

(†) N.M. Barysheva et al. Comput. Math. Math. Phys. **22**, 156 (1982);
A.I. Zuev, Comput. Math. Math. Phys. **32**, 70 (1992).

Modified version of 1D ERA hydrocode…

$$W_{e,i} = -\kappa_{e,i} \cdot \rho \cdot \frac{\partial T_{e,i}}{\partial \mathrm{q}},$$

$$\kappa_i = 0, \quad \kappa_e = \alpha \frac{(\theta_e^2 + 0.16)^{5/4} \cdot (\theta_e^2 + 0.44)}{(\theta_e^2 + 0.092)^{1/2} \cdot (\theta_e^2 + \beta \cdot \theta_i)} \cdot \theta_e,$$

$$\theta_e = T_e / E_F, \quad \theta_i = T_i / E_F, \quad \alpha = 377 \ \frac{\mathrm{W}}{\mathrm{m} \cdot \mathrm{K}}, \ \beta = 0.139$$

J.P. Colombier et al. PRB, **71**, 165406 (2005).

Modified version of 1D ERA hydrocode…

Electron-ion exchange term:

$$\Delta Q_{ei} = \gamma \cdot \left(T_e - T_i\right),$$

$$\gamma = \gamma_{\mathrm{pl}} = \frac{3 m_e k_B}{m_i^2} \nu_{e,i} \ (\dagger); \quad \gamma = \gamma_{lat} = \frac{\pi \hbar k_B \lambda \left\langle \omega^2 \right\rangle}{g\left(E_F\right)\rho} \int\limits_{-\infty}^{+\infty} g^2\left(\varepsilon\right)\left(-\frac{\partial f}{\partial \varepsilon}\right) d\varepsilon \ (\ddagger),$$

$$g\left(\varepsilon\right) - \mathrm{DOS}, \ f\left(\varepsilon, \mu, T_e\right) = \left\{\exp\left[\left(\varepsilon - \mu\right)/k_B T_e\right] + 1\right\}^{-1};$$

$\left\langle \omega^2 \right\rangle$ – second moment of the phonon spectrum,

λ – electron-phonon mass enhancement parameter.

(†) K. Eidmann et al. PRE, **62**, 1202 (2000).
(‡) Z. Lin, L.V. Zhigilei, and V. Celli. PRB, **77**, 075133 (2008)

Modified version of 1D ERA hydrocode…

Effective frequencies of e-i and e-e collisions in broad temperature range — use harmonic-mean interpolation between cold-metal & high-temperature (Spitzer) frequencies (Eidmann, 2000; Fisher, 2001):

$$\nu_{ei} = (\nu_{Sp}^{-1} + \nu_{e,ph}^{-1})^{-1},$$

$$\nu_{Sp} = \frac{4}{3}\sqrt{2\pi}\,\frac{\langle Z\rangle e^4 m_e n_e}{(m_e k_B T_e)^{3/2}}\ln\Lambda, \quad \nu_{e,ph} = k_s \frac{e^2 T_i}{\hbar^2 \mathrm{v}_F},$$

$$(\mathrm{v}_F \ll c,\ \hbar\omega_{pi} \ll k_B T_i)$$

$$\nu_{e,e} = (1/\nu'_{ee} + 1/\nu''_{ee})^{-1},$$

$$\nu'_{e,e} = \frac{E_F}{\hbar}\left(\frac{T_e}{E_F}\right)^2 \ @\ T_e/E_F \le 1, \quad \nu''_{e,e} = \frac{E_F}{\hbar}\left(\frac{T_e}{E_F}\right)^{-3/2} \ @\ T_e/E_F \ge 3.$$

K. Eidmann et al. PRE, **62**, 1202 (2000); D. Fisher et al. PRE, **65**, 016409 (2001).

Modified version of 1D ERA hydrocode…

Absorption of s- and p-polarized laser light — Maxwell equations with (complex) Drude dielectric function:

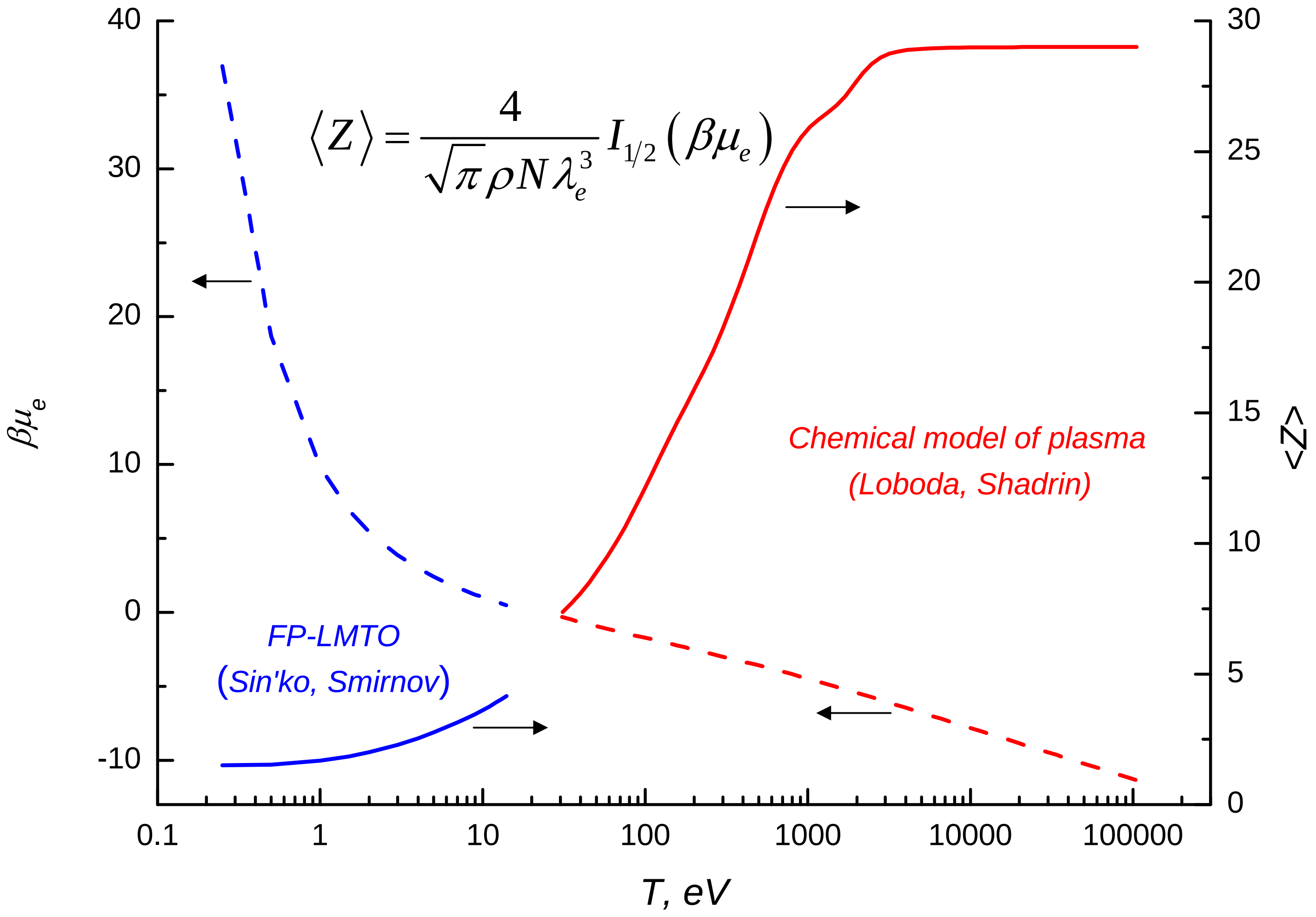
$$\frac{d^2E(z)}{dz^2}+k^2\left(\varepsilon-\sin^2\theta\right)E(z)=0,$$

$$\frac{d^2B(z)}{dz^2}+k^2\left[\varepsilon-\sin^2\theta\right]B(z)-\frac{d\ln\varepsilon}{dz}\cdot\frac{dB(z)}{dz}=0,$$

$$\varepsilon=1-\frac{\omega_{pe}^2}{\omega_L\left(\omega_L+i\nu_{eff}\right)},\quad \omega_{pe}^2=\frac{4\pi e^2n_e}{m_e},\quad \nu_{eff}=\nu_{ei}+\nu_{ee}.$$

Thermodynamics with FP-LMTO & CP-models

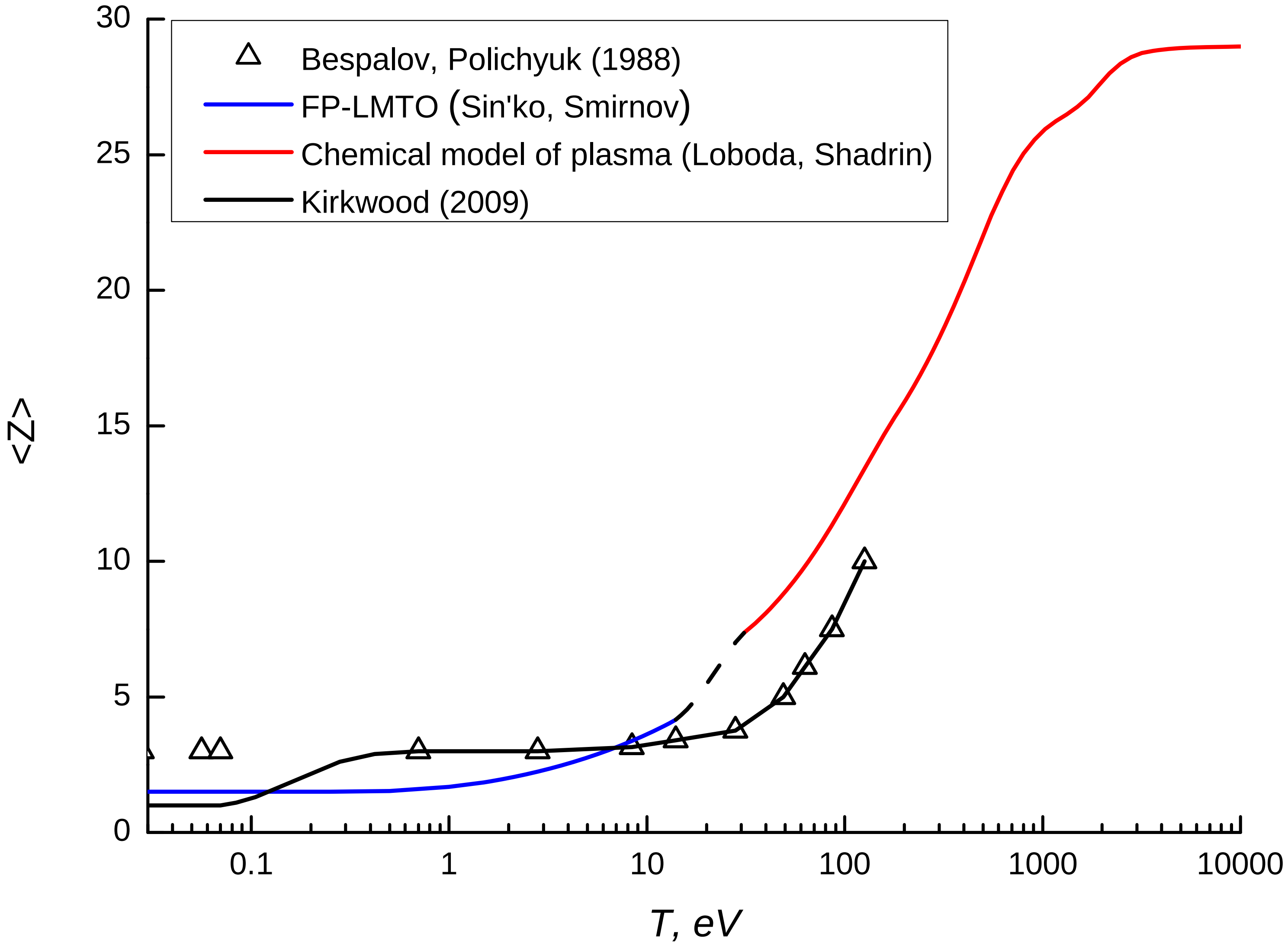
$\mu(T_e)$ and $\langle Z\rangle$ of solid-density Cu:



$$\langle Z\rangle = \frac{4}{\sqrt{\pi}\,\rho N \lambda_e^3} I_{1/2}\left(\beta\mu_e\right)$$

P.A. Loboda, V.V. Popova, A.A. Shadrin. Contrib. Plasma Phys., **49**, 738 (2009).

Thermodynamics with FP-LMTO & CP-models…



I.M. Bespalov, A.Ya. Polishuk. Preprint IVTAN № 1-257. (1988).

Thermodynamics with FP-LMTO & CP-models…

Dielectric permittivity of solid-density Cu

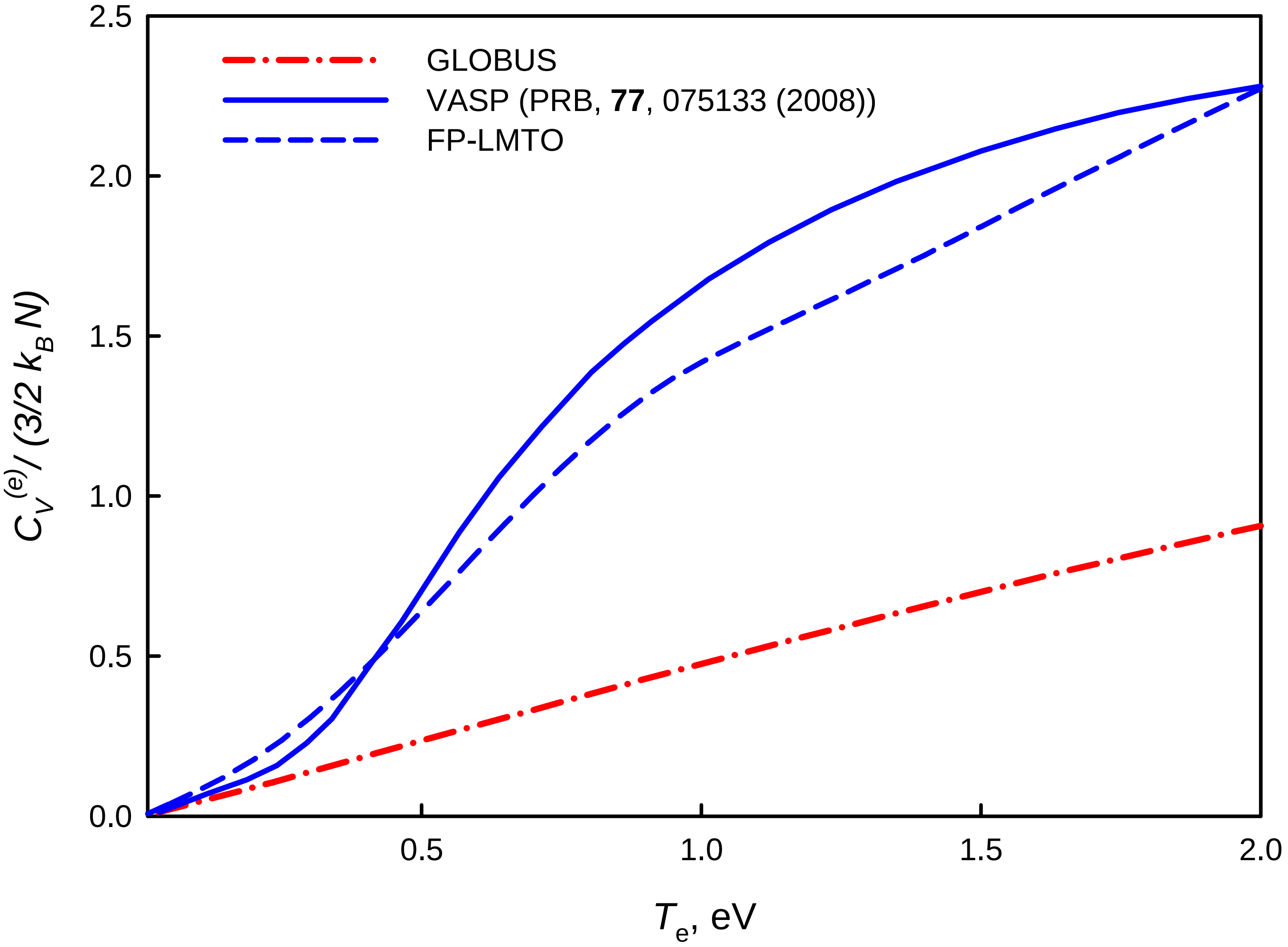
$\varepsilon_{\text{cold Cu}} = -27 + 2.5i$ is reproduced in the ERA simulations @ the accuracy of 20% with $k_s = 5.3$ in $\nu_{\text{e, ph}}$

Electron plasma frequency of solid-density Cu

@ $T_e \leq E_F$ is interpolated from high-temperature $\omega_{p,e}$ to the value directly yielded by FP-LMTO calculations => no effective electron mass used in the ERA simulations

Thermodynamics with FP-LMTO & CP-models…

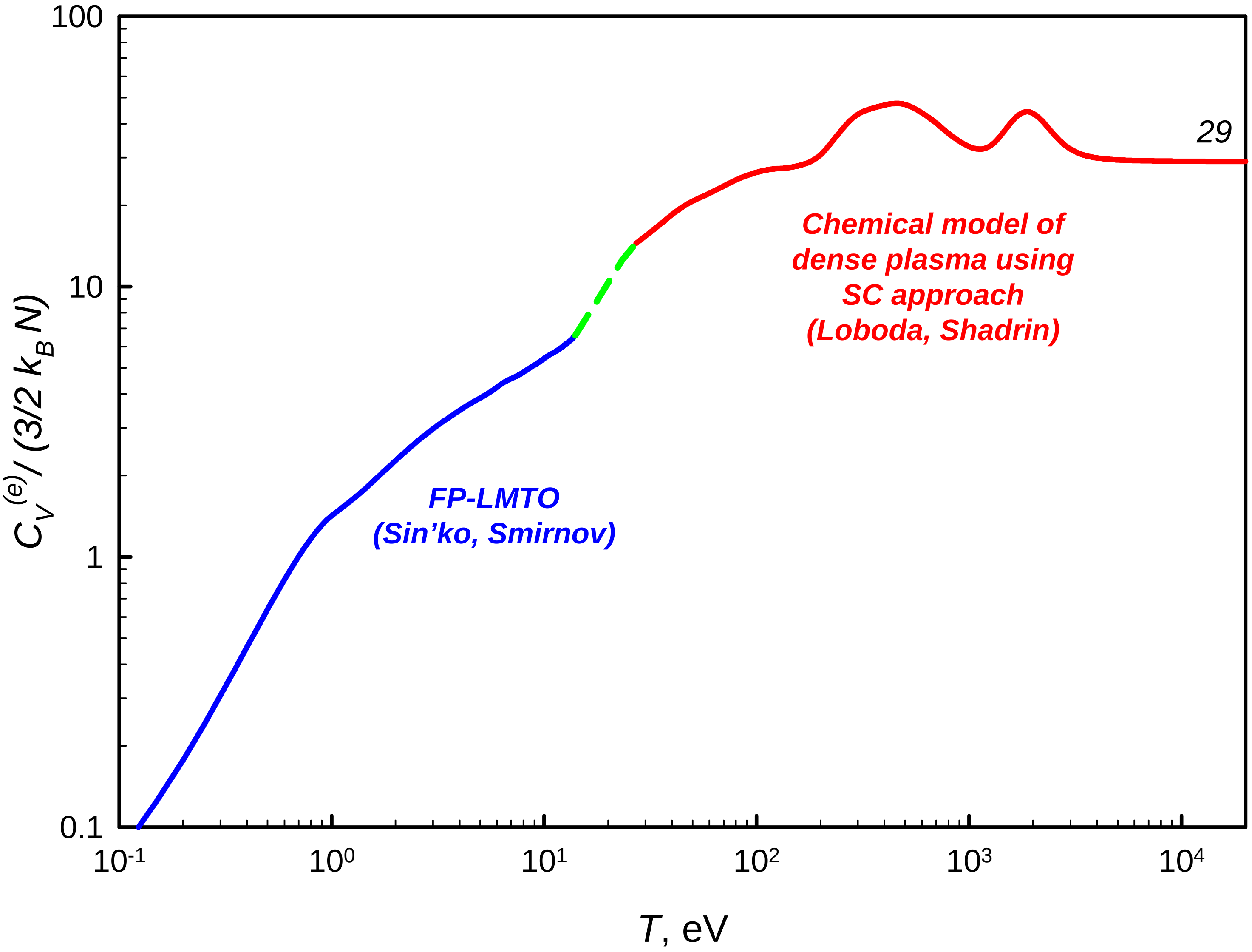
Electron specific heat of solid-density Cu:



A.T. Sapozhnikov et al. VANT, Ser.: Math. Mod of Phys. Proc, **1**, 9 (1991).

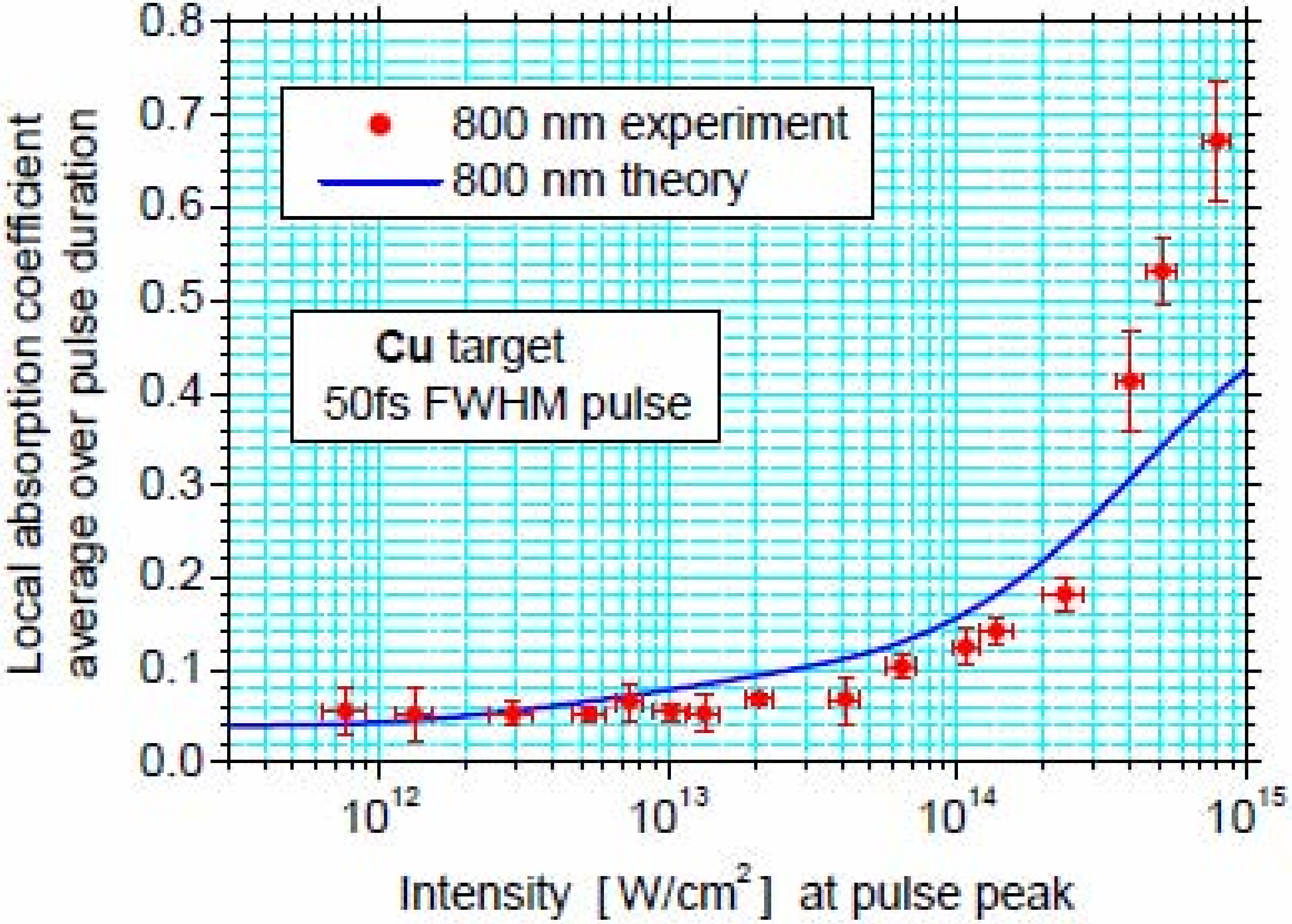
Thermodynamics with FP-LMTO & CP-models…

Wide-range electron specific heat of solid-density Cu



Comparisons to experimental and other theoretical data

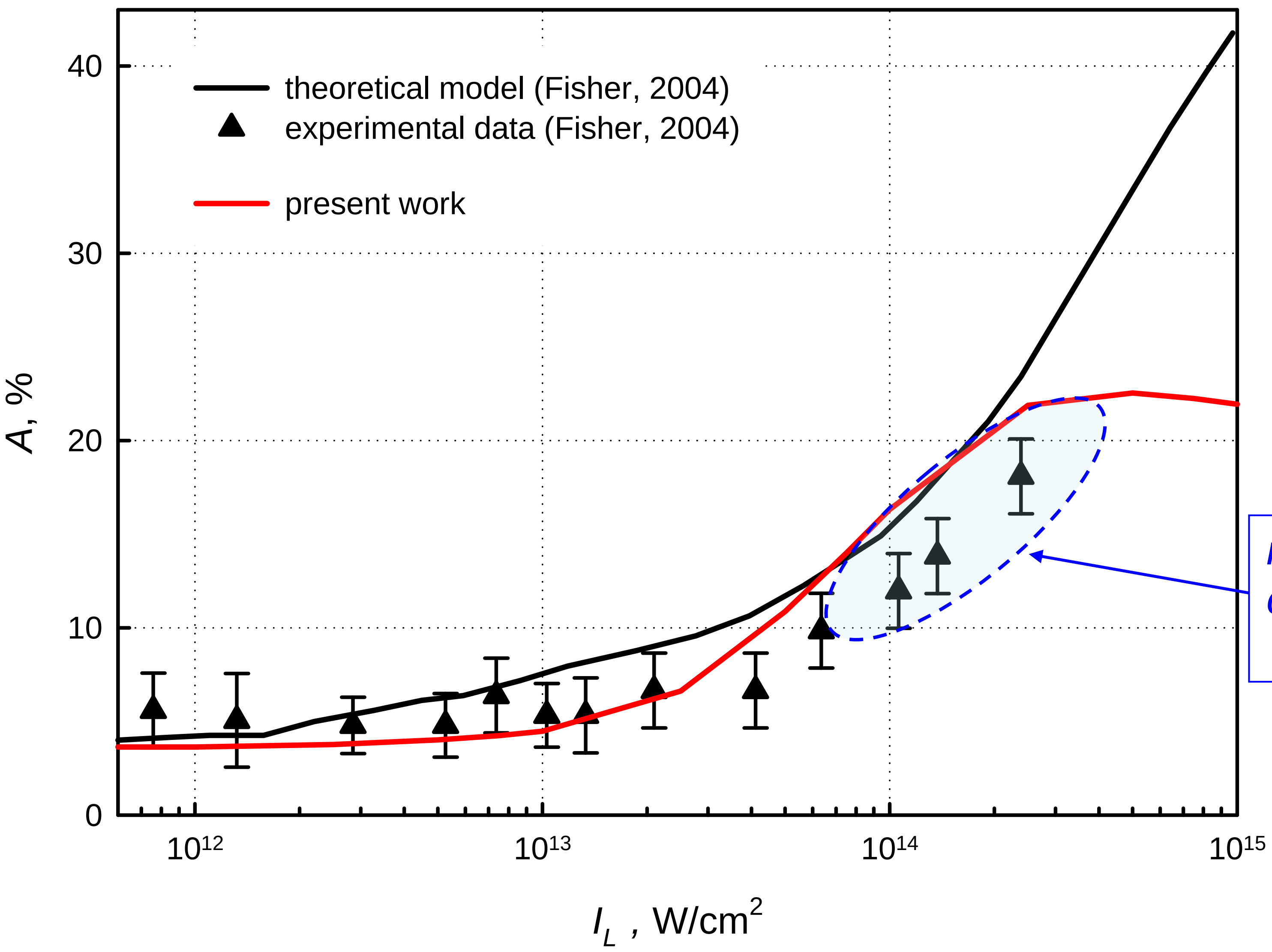
Absorption of 50-fs 1ω Ti:Sa-laser pulses in Cu targets



D. Fisher et al. Proc. XXVIII ECLIM (2004).

Comparisons to experimental and other theoretical data

$\theta = 0,\ \tau_L = 50\ \text{fs},\ \lambda_L = 800\ \text{nm}$



more accurate calculation of ν_{ee} is needed

Absorption of Ultrashort Laser Pulses by Solid Targets Heated Rapidly to Temperatures 1–1000 eV

D. F. Price, R. M. More, R. S. Walling, G. Guethlein, R. L. Shepherd, R. E. Stewart, and W. E. White
Lawrence Livermore National Laboratory, Livermore, California 94550

(Received 4 April 1995)

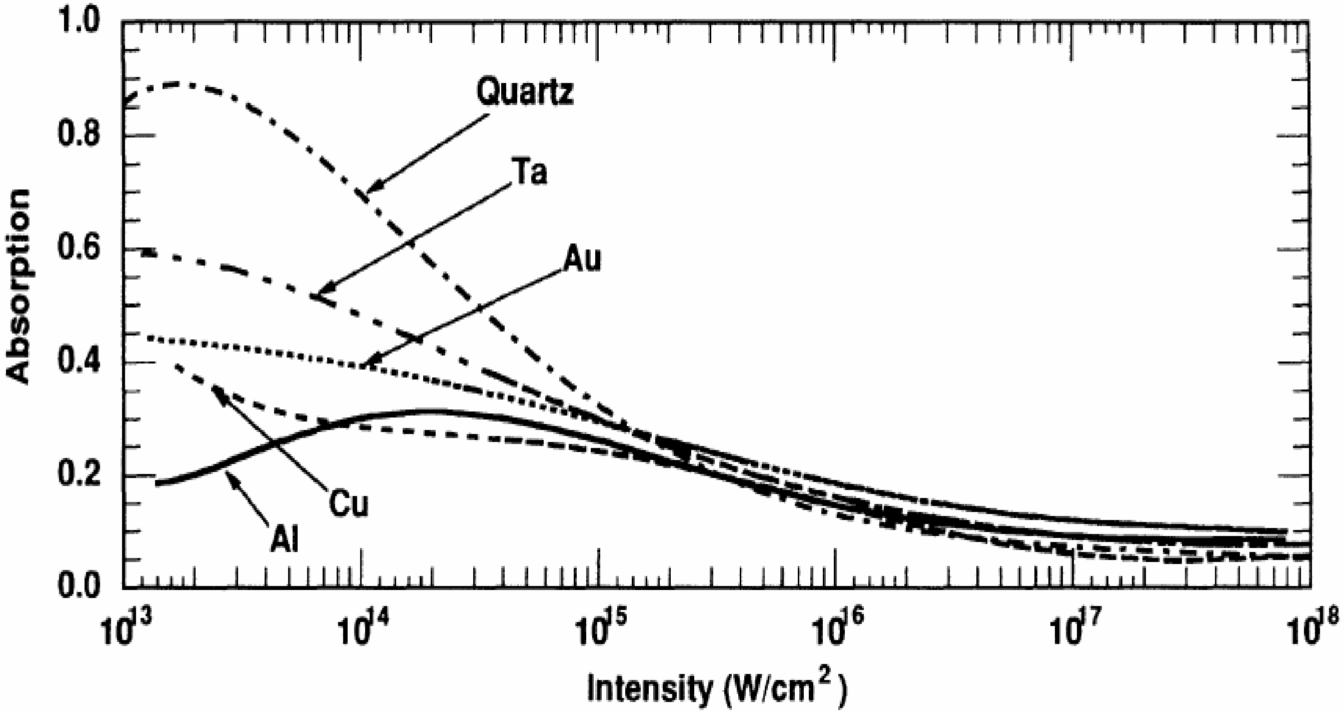


FIG. 1. Absorption fraction vs peak laser intensity for aluminum, copper, gold, tantalum, and quartz targets. In Figs. 1, 3, 4, and 5 laser intensity is the temporal and spatial peak value of the laser intensity.

Conclusions

- Simulations of absorption of normal-incident femtosecond laser pulses in copper using modified ERA hydrocode have been done.
- Thermodynamic functions calculated by using FP-LMTO & CP-model of dense plasma utilizing SC approach bring the ERA simulations into a very good agreement with experiment @ $I_L \leq 7\times10^{13}$ W/cm^2. Increasing deviations from the experiment (prepulse?) & previous modeling (transition to plasma-mirror behaviour?) are found @ $I_L \geq 10^{14}$ W/cm^2
- more accurate calculation of ν_{ee} & comparisons to other theoretical data are needed.

Thank you

for your attention!