

# Non-Equilibrium Modeling of Warm Dense Matter

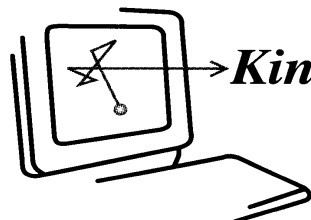
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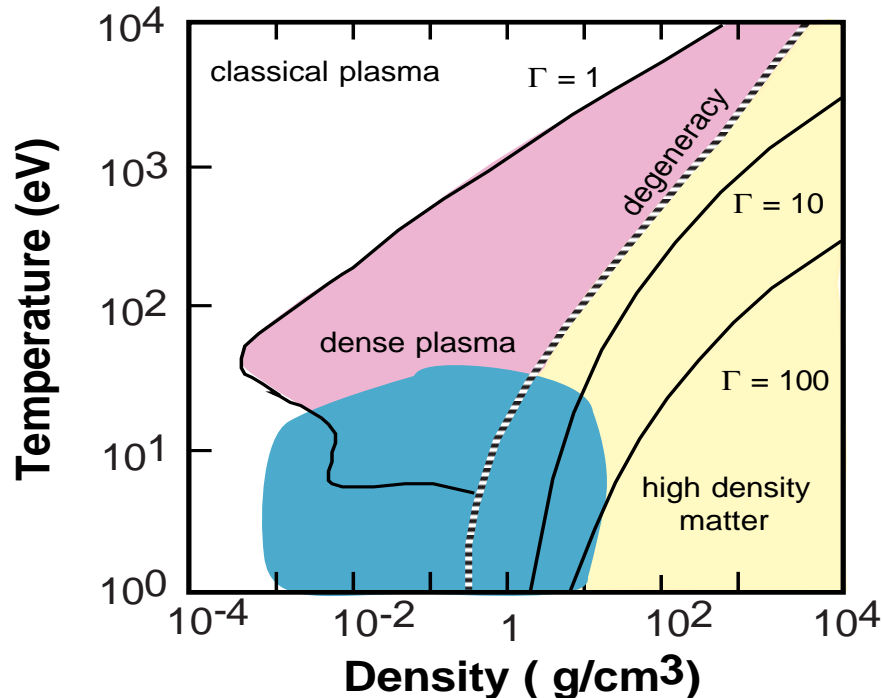
# Introduction

- We are developing physics models and codes for investigation of highly non-equilibrium plasmas on time scales of tens of femtoseconds, electron temperatures in 1-10 eV range, and cold ions near solid density
- Such *Warm Dense Matter (WDM)* plasmas will be produced by high brightness, hard x-ray free electron lasers currently under development

# Warm Dense Matter (WDM) regime is just beginning to be explored

**WDM is the region in temperature (T) - density ( $\rho$ ):**

- 1) Not described as normal condensed matter, *i.e.*,  $T \sim 0$
- 2) Not described by weakly coupled plasma theory



- $\Gamma$  is the strong coupling parameter, the ratio of the interaction energy between the particles,  $V_{ij}$ , to the kinetic energy,  $T$

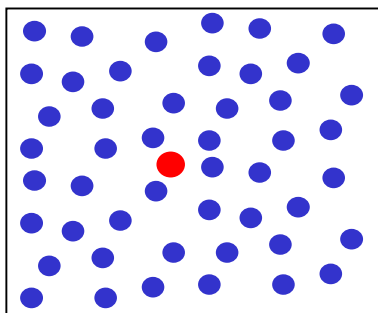
- $$\Gamma = \frac{V_{ii}}{T} = \frac{Z^2 e^2}{r_o T}$$

where  $r_o \propto \frac{1}{\rho^{1/3}}$

# From the point of view of a plasma the defining concept is coupling

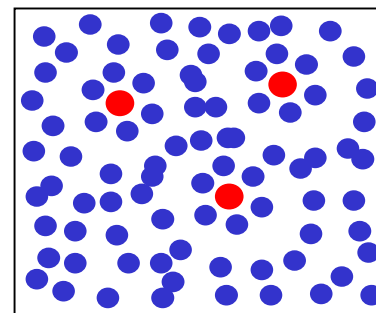
- **Weakly coupled plasmas are easy**

- The plasma can be seen as a separate point charges
- Then the plasma is a bath in which all particles are treated as points - even particles with structure (*e.g.*, atoms)



as T decreases

or density increases



- **But, when either  $r$  increases or  $T$  decreases  $\Gamma > 1$ :**

- Particle correlations become important
- Ionization potentials are depressed
- Energy levels shift

# A novel approach is needed for these novel states of matter required

## One has:

- a highly transient system
- a strongly non-Maxwellian electron distribution,
- electrons coupling with the initially structured solid density material

## One must:

- Use non-LTE atomic population kinetics code integrated with Boltzmann equation solver

## One will obtain:

- a self-consistent time-dependent solution of the level populations and the particle energy distributions
- ionization balance and the spectral output of transient systems electron distributions

## Ct27 : FLYCHK & Zelda

# Boltzmann's Equation for Non-LTE electrons

$$\frac{\partial n_e(\varepsilon)}{\partial t} = \left[ \frac{\partial n_e(\varepsilon)}{\partial t} \right]_{\text{Elastic}} + \left[ \frac{\partial n_e(\varepsilon)}{\partial t} \right]_{\text{Inelastic \& Superelastic}} + \left[ \frac{\partial n_e(\varepsilon)}{\partial t} \right]_{\text{Sources}} - \left[ \frac{\partial n_e(\varepsilon)}{\partial t} \right]_{\text{Sinks}} + \left[ \frac{\partial n_e(\varepsilon)}{\partial t} \right]_{\text{Electron - Electron}}$$

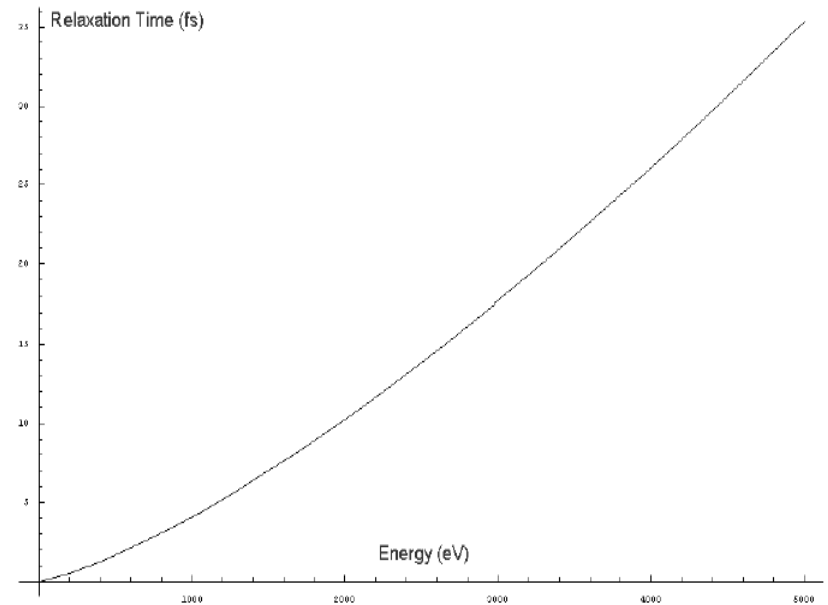
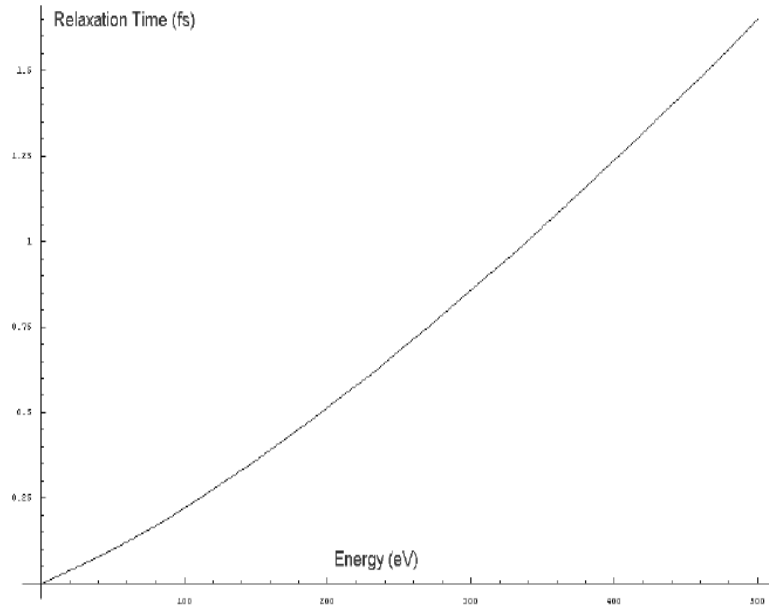
where  $n_e(\varepsilon) = N_e \varepsilon^{1/2} f(\varepsilon)$  and  $\int d\varepsilon f(\varepsilon) \varepsilon^{1/2} = 1$

**The terms are:**

- Elastic losses to phonon (deformation potential) scattering
- Inelastic (excitation) and superelastic (de-excitation) of bound states
- Sources such as photo- and Auger electrons
- Sinks such as 3-body, dielectronic, and radiative recombination
- Electron thermalization due to collisions with other electrons

# Non-Maxwellian electron distribution will be important to system evolution

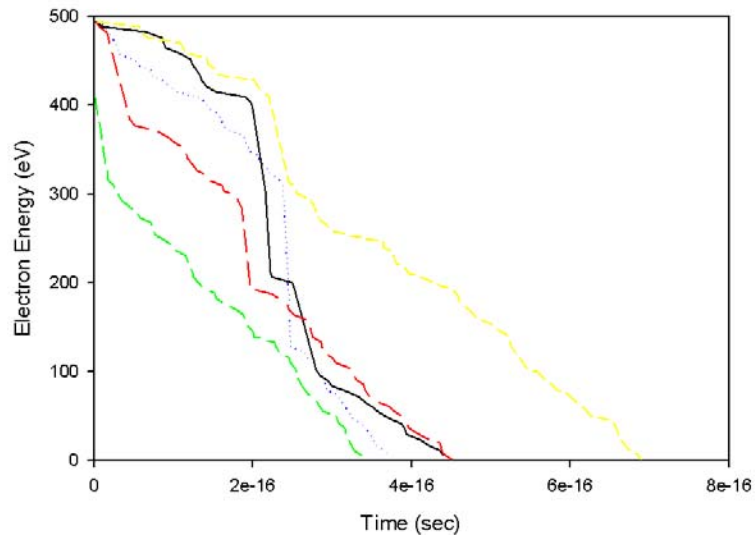
The **energy loss time** for the high energy electron interacting with the relatively cool background electron gas is comparable to the **pulse duration time**



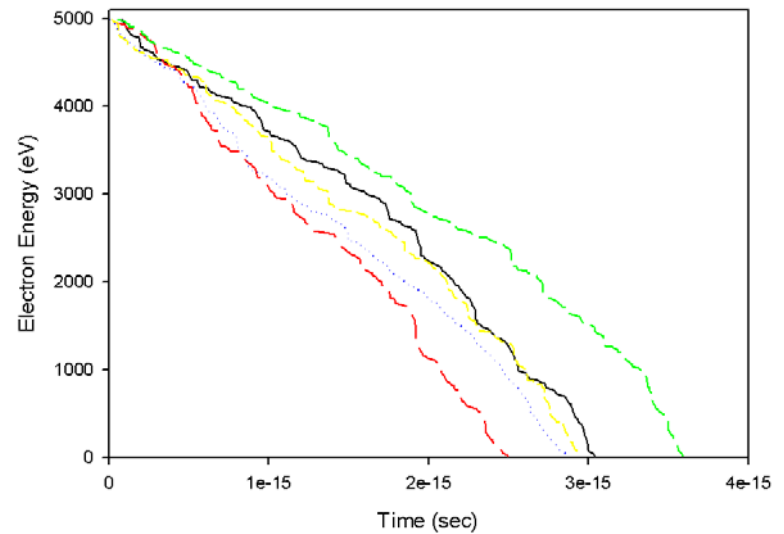
# Relaxation time due to inelastic collisions

$\tau_{\text{inelastic}} \ll \tau_{\text{electron-electron}}$  leads to non-Maxwellian electron distributions

Five Random Walks in Energy Space  
Starting at 500 eV



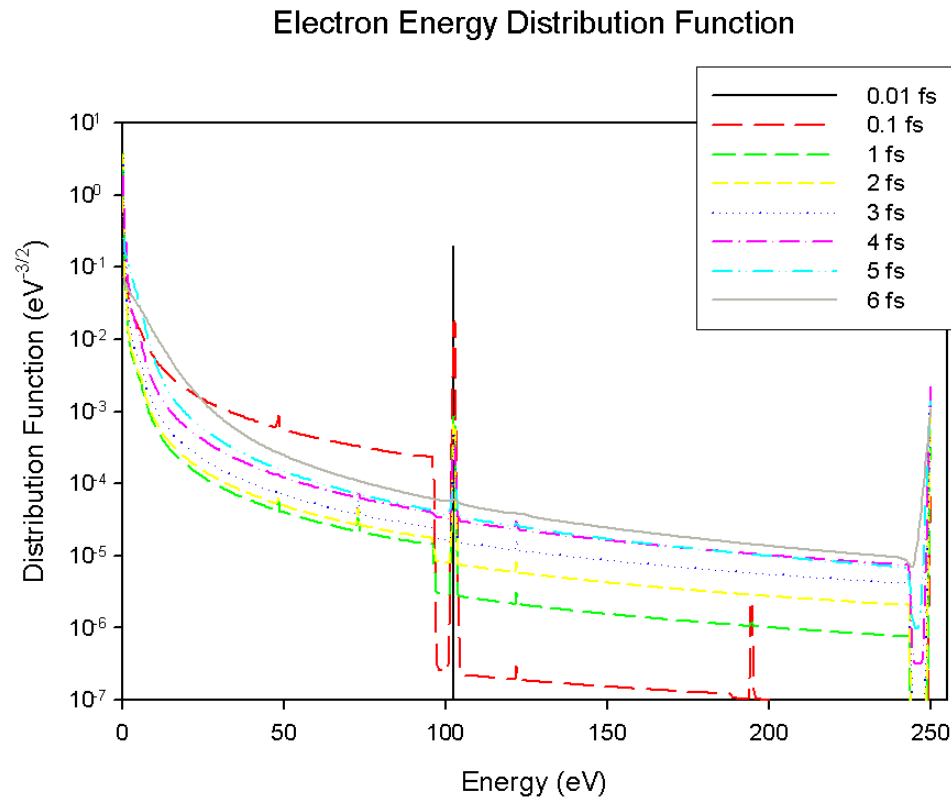
Five Random Walks in Energy Space  
Starting at 5 keV





# Time Evolution of $f(\varepsilon)$

Al plasma driven by x-ray photo & Auger ionization



# Work in Progress

Development of modeling codes and addressing physics issues in parallel with the development of x-ray FEL light sources.

## References:

Lee, et al., *Laser & Particle Beams* **20**, 527 (2002)

Lee, et al., *JOSA B* **20**, 770 (2003)

TESLA FEL Technical Design Report [http://tesla.desy.de/tdr\\_update](http://tesla.desy.de/tdr_update)

# Path is defined by proposed facilities and each requires development $\Rightarrow$ 5 year plan

## •Develop experiments on short pulse lasers and 3<sup>rd</sup> generation light source facilities

- Provides time resolution of  $\sim 100$  fs
- Provides method to develop FTDM experiments

## •Develop experiments for DESY TTF-II

- Provides high peak brightness for potential heating and/or 200 fs probing

## •Develop experiments for LCLS/TESLA X-FELs

- Provides harder x-ray capability at high peak brightness
- 200 fs probing and x-ray heating

Peak Brightness vs. Energy for present and future x-ray sources

