Non-Equilibrium Modeling of Warm Dense Matter

56th Gaseous Electronics Conference (www.gec.org)

San Francisco, CA October 2003

Hyun-Kyung Chung
Lawrence Livermore National Laboratory
hchung@llnl.gov

W. L. Morgan
Kinema Research, Monument, Colorado
morgan@kinema.com

Richard W. Lee
Lawrence Livermore National Laboratory
dicklee@physics.berkeley.edu

Kinema Research & Software, L.L.C.
719.481.1305 • Fax: 719.481.1398
P.O. Box 1147 • Monument, CO 80132

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

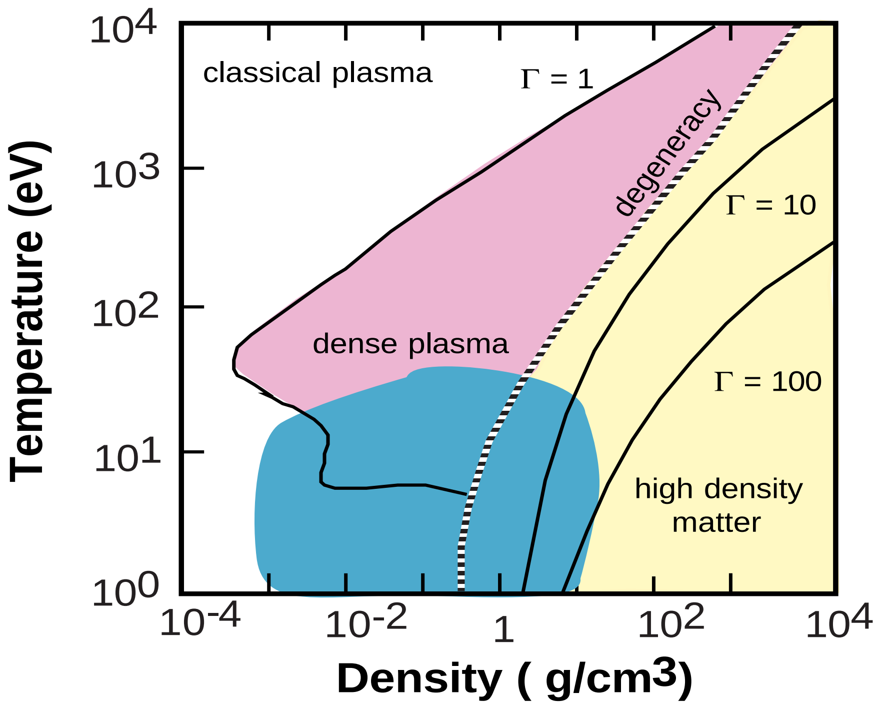
• Such *Warm Dense Matter (WDM)* plasmas will be produced by high brightness, hard x-ray free electron lasers currently under development

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

WDM is the region in temperature (T) - density (ρ):

1) Not described as normal condensed matter, *i.e.*, T ~ 0

2) Not described by weakly coupled plasma theory



- Γ is the strong coupling parameter, the ratio of the interaction energy between the particles, V_{ii}, to the kinetic energy, T
-

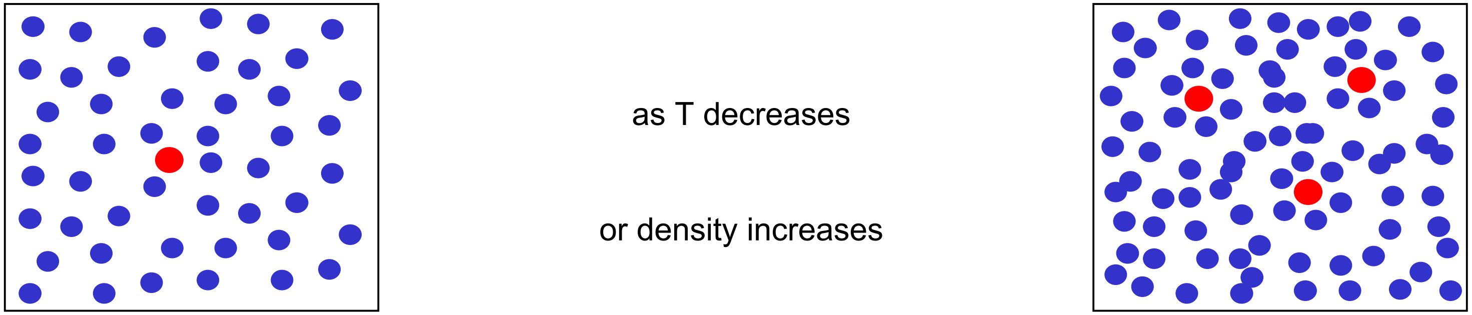
$$\Gamma = \frac{V_{ii}}{T} = \frac{Z^2 e^2}{r_o T}$$

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

Kinema Research & Software

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)



- **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

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

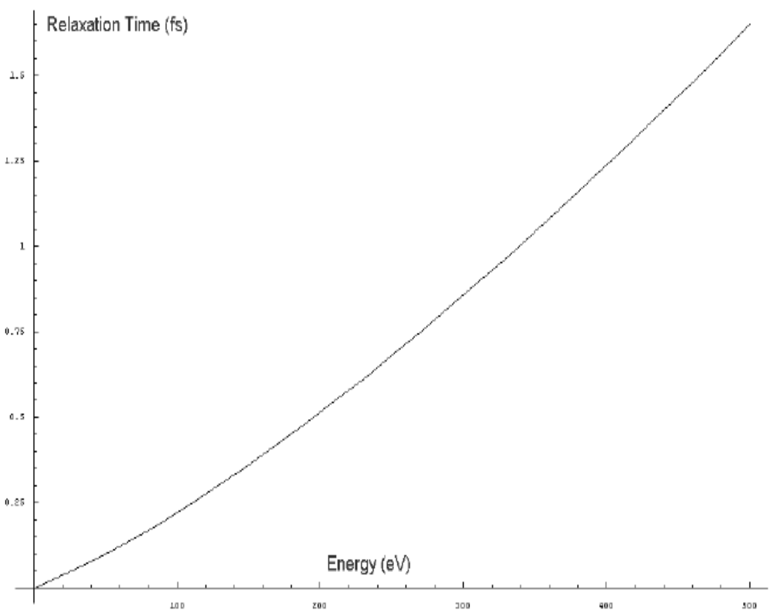
where $n_e(\varepsilon) = N_e \varepsilon^{1/2} f(\varepsilon)$ and $\int d\varepsilon f(\varepsilon)\varepsilon^{1/2} = 1$

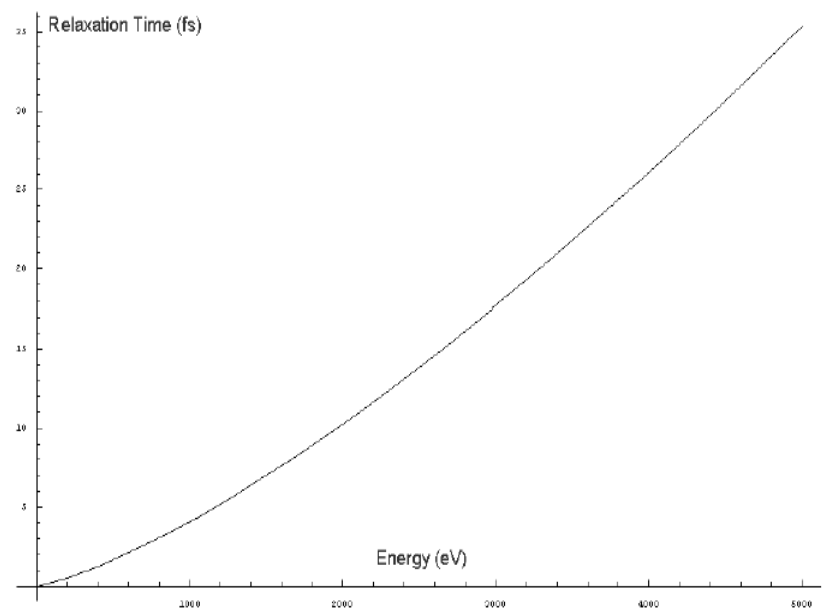
The terms are:

- 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

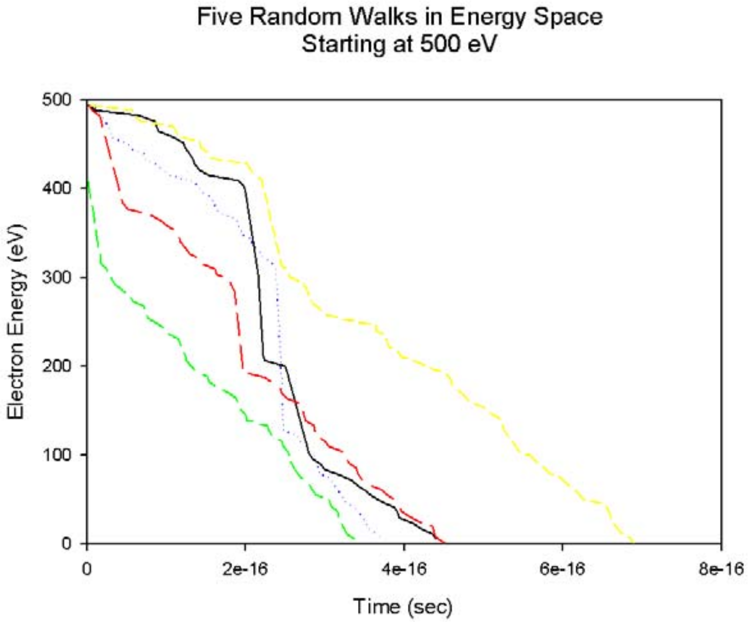
The energy loss time for the high energy electron interacting with the relatively cool background electron gas is comparable to the pulse duration time

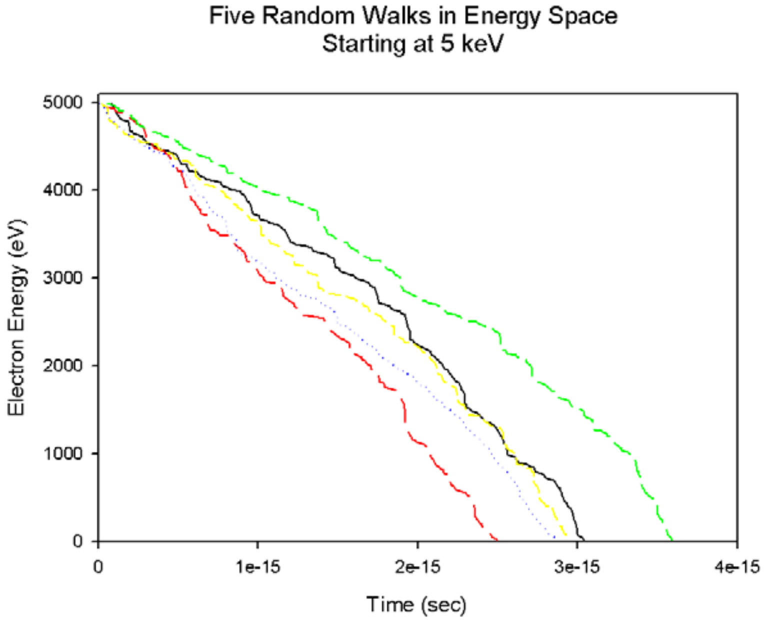




Relaxation time due to inelastic collisions

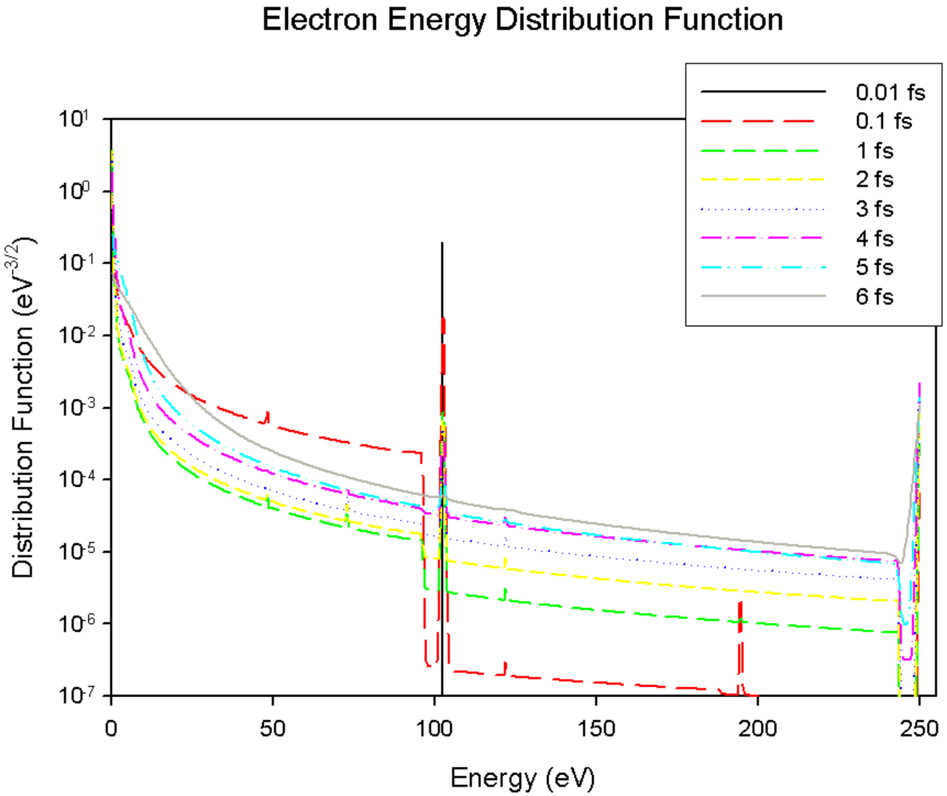
$\tau_{inelastic} << \tau_{electron\text{-}electron}$ leads to non-Maxwellian electron distributions





Time Evolution of f(ε)

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*

Path is defined by proposed facilities and each requires development ⇒ 5 year plan

•Develop experiments on short pulse lasers and 3rd generation light source facilities

•Provides time resolution of ~ 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