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HIGH ENERGY DENSITY PHYSICS - PHYSICS & MODELLING[1]

S. V. G. MENON

CONTACT INFORMATION:

e-mail: menonsvg@yahoo.co.in

e-mail: menon.svg98@gmail.com

mobile: +918879394488

mobile:+918547992824

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High Energy Density Systems – Physics & Modelling

S. V. G. MENON

Abstract

Physics of high energy density (HED) systems finds applications in several fields of current research: astrophysics, Inertial Confinement Fusion (ICF), pulsed power systems, impact phenomena, etc. Theoretical study of this field involves modelling various physical processes such as fission and fusion physics, hydrodynamics and shockwaves, radiation and explosive driven phenomena, transport of neutral and charged particles, radiation transport, and growth of hydrodynamic instabilities. To achieve this, one requires various databases of material properties, which are supplemented by accurate theoretical modelling. The databases include thermodynamic properties of matter in wide ranges of conditions, radiation transport properties of materials, neutral and charged particle interaction cross-sections, and detonation properties of high explosives.

HED systems occurring in ICF are of particular interest. A comprehensive approach to ICF requires integration of all the physical processes in simulations and development of methods validated with experiments. As experiments in this field are severely limited to narrow ranges of thermodynamic conditions, detailed simulations can only provide sufficient insight. This article presents theoretical models and simulation studies of some of the processes involved [1]

I. Introduction

Matter under extreme conditions of temperature and pressure occur in several fields (see Table-I). Recent scientific and technological advances are making it possible to study these systems at a fundamental level in the laboratory. This article is concerned about the underlying physical phenomena at rather high energy density (HED) occurring in these systems, theoretical modelling, and the need for computer simulations.

Table-I: High Energy Density Systems	
1. Inertial Confinement Fusion Devices	4. High Current Driven Devices
2. Explosive & Impact Loading of Materails	5. Geophysics & Planetary Interiors
3. Nuclear Weapons	6. Astrophysics – Stellar Objects

HED systems are typically those subjected to pressures in excess of 1Mbar (1 million atmospheres). This range of pressure is equivalent to 10^5 J/cm^3 of internal energy density. Energy density of this order corresponds to dissociation of a hydrogen molecule. At these conditions, all matter becomes compressible as well as ionisable and hence would exist in the plasma state. In most situations, the plasma is very dense and has properties quite different from those of dilute plasmas, which are described by classical plasma theory.

High energy density physics (HEDP) deals with the properties of matter existing in systems as shown in Table-I. In the first four cases, matter passes different states through various phase transitions during the dynamical course of reaching the final condition. Detailed knowledge of thermodynamic properties is necessary to understand the evolution of these systems. Experiments required to generate HED conditions are quite difficult due to limited spatial, temporal and energy scales achievable in the laboratory. In other words, the ranges of parameters, which can be covered in experiments, are rather narrow. Therefore, modelling and simulations are integral parts of HEDP.

Inertial confinement fusion/fission (ICF) devices are, perhaps, the most prominent of all HED systems. This is so due to their potential for utilization of nuclear energy. ICF physics has significant overlap with nuclear weapons physics. Though the states of matter produced and physical processes involved are similar, the characteristic scales in the two cases are quite different. In this article, we will be mainly concerned with the physics of ICF devices.

Current research in ICF are focused on interaction of laser and particle beams with matter, dynamics of X-rays in hohlraums, hydrodynamic instabilities in implosions, ablator physics, different schemes of thermonuclear ignition and burn. We are developing theoretical and computational models for simulation of these phenomena. This is being pursued via four complementary paths: (i) inclusion of the fine details of physical process; (ii) development of fast and efficient numerical algorithms; (iii) use of modern visualization tools, and finally, (iv) parallelization of some of the codes for utilizing large computer resources.

The article proceeds with a definition of HED regime, physics of ICF devices, methods of generating HED conditions and brief discussion of various physical processes involved.

II. Defining HED regime

The energy densities occurring in commonly known systems like capacitors to fission and fusion devices are compared in Table-II. These can be classified as steady state and dynamical systems. The table gives an idea of the energy densities involved in HED systems. Since the time scales involved in these devices are quite different, it is also necessary to compare the typical power levels at which these systems operate.

Table-II: Energy Density (kJ/kg) in Various Devices	
Capacitors	0.022
Explosives	5×10^3
Fission Devices	9×10^7
Fusion Devices	3×10^8
Stellar Objects	1×10^6

Table-III: Typical Power Generation in Systems				
Steady State Systems		Dynamic Systems		
Automobile	50-200 kW	High Power	10^{14} W	time ~ 1ns
Energy from Sun	4×10^{26} W	Explosives (1Kg)	10^{12} W	time ~ 1μs
Nuclear Reactors	10^{9} W(e)	Fission Device	10^{22} W	time ~ 0.25μs

While complete burning of 1 kg of chemical explosive produces about 5 MJ at 10^{12} Watt, total fission of 1 kg of U^{235} provides 17.6 kT (1 kT = 10^{12} Calories) of energy at about 10^{22} Watt. Fusion of 1 kg of equal mixture of D-T gives rise to 80.4 kT of energy which is more than 4 times the specific energy in fission.

We next turn to Fig. 1 showing the HED regimes for hydrogen in terms of a density-temperature plot [2]. The scales involved are quite large as it covers 20 orders in density and 9 orders in temperature. On the lowest density side, going up on temperature, there is a grey line separating un-ionized and ionized hydrogen. This line has a positive initial slope with density, however, it drops down later, and after about 1g/cc, hydrogen is found to be ionized at all temperatures. This is termed as pressure ionization. The horizontal lines marked P (total) = 1Mbar and 1Gbar denote contours of radiation pressure that do not depend on material density. Above these lines, radiation pressure would dominate material pressure. The slanting lines marked P (gas) = 1Gbar and 1Mbar are contours of total pressure. Thus, thermal pressure in hydrogen at 1 g/cc density and 1 eV temperature (1.16 x 10^{4} K) is about 1Mbar.

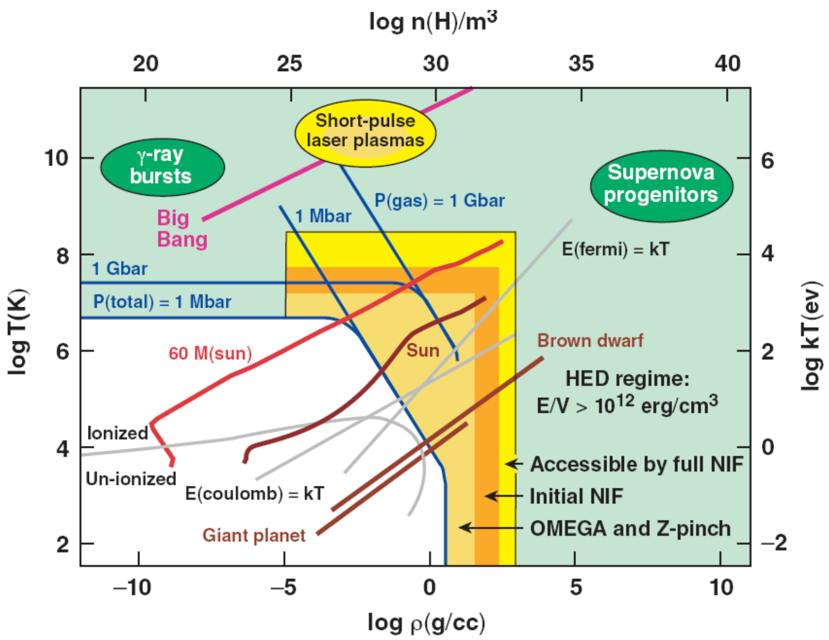

Fig. 1: Density-Temperature regimes in HED systems

Below the line "E (Coulomb) = kT", thermal energy of plasma is less than Coulomb energy, which means that the plasma is strongly coupled. Similarly, below the line "E (Fermi) = kT", plasma is no more classical and the quantum mechanical Fermi-Dirac pressure overwhelms thermal pressure. There are lines moving from low to high density depicting the time development of giant planets, brown dwarfs, Sun, a star of 60 solar mass, and big bang explosion. Regions showing γ-ray bursts and supernova progenitors are of great astrophysical significance. The area indicated as short pulse laser plasma are being studied using table-top lasers that generate pulses of ~ 10^{-15} sec. Coloured regions accessible to laser facilities like OMEGA & Z-pinch, initial National Ignition Facility (NIF), USA, and the full NIF indicate that experimentation is feasible over very limited regions only. As mentioned earlier, this brings in the need for theoretical modelling and simulations of these systems. The models have to be robust as well as accurate. Next, we turn to the basic processes involved in ICF.

III. Inertial Confinement Fusion/Fission

ICF has driven much of the development of HED physics. Though there is ample literature on fusion devices, fission of micro fissile targets is also possible using the same principles. The fusion target, which is a capsule containing equal mixture of D-T, is a complex structure designed to produce energy when driver beams are shone on it. A material called ablator (for example, Be) covers the target. Laser beams are employed as driver for direct drive scheme. Several laser beams (see Fig. 2) impinge on the target and generate an ablating plasma, which implodes the fuel to conditions appropriate for initiating thermonuclear fusion.

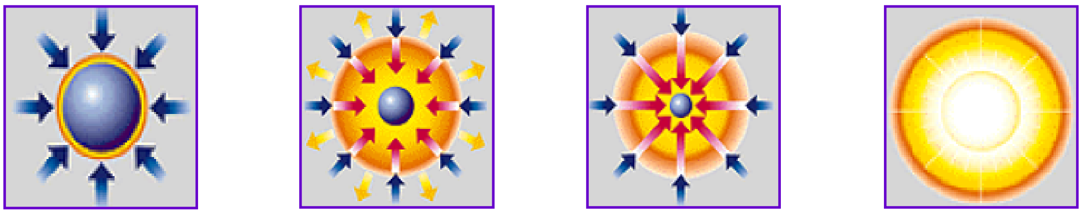

Fig. 2: Extreme pressures generated via ablation compresses D-T fuel to ignition. (L – R): (i) ablation, (ii) implosion, (iii) ignition, and (iv) burn.

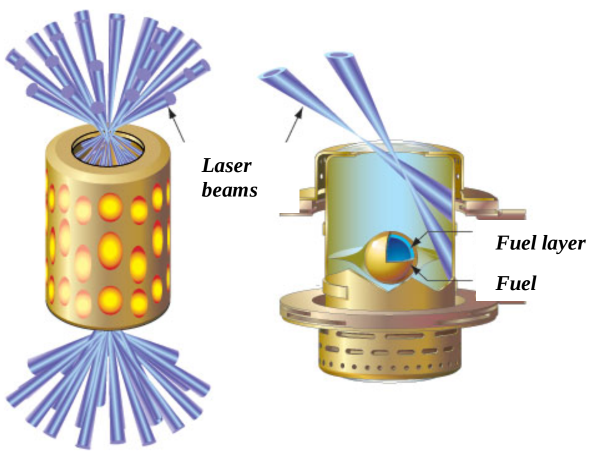

Fig. 3: In indirect drive, energy from laser beams is converted to X-rays inside the hohlraum. Uniformity of X-rays reduces asymmetries inherent in direct drive.

In indirectly driven scheme, the drivers can be lasers, particle beams, or electron beams. Energy from the driver (see Fig. 3) is converted into thermal X-rays in a hohlraum, which is made of high-Z material like Au or U. Typical temperature of thermal X-rays is 250 eV. The X-rays absorbed by capsule generates a hot plasma, which ablates outwardly. The reaction force accelerates the remaining fuel inwards leading to compression and heating of the fuel to high temperature. Energy transport in the hohlraum via radiation is an essential feature here.

IV. Creating conditions of HED

Gravitational forces generate HED conditions in nature, for example, pressures at the centre of Earth and Jupiter are about 4 Mbars and 40 Mbars, respectively. Gravity also holds steller matter together leading to conditions suitable for thermonuclear fusion. Pressure at the core of the Sun is, approximately, in the range of trillion bars.

HED conditions have been realized in the laboratory with the advent of modern technology. Mainly five methods are pursued in different laboratories. These include: (i) explosive driven impact pheneomena, (ii) direct irradiation with laser, (iii) X-rays from laser driven hohlraums, (iv) Z-pinch and related pulsed power devices, and (v) irradiation with electron and ion beams. All these are dynamic experiments. Driver energy is deposited in a small region at extremely fast rate leading to the formation and propagation of shock waves.

1. Experimental Systems:

Laser Facilities: NIF employs neodymium-glass laser system with 192 beams which can deliver as much as 2 MJ of laser energy (of wavelength 0.35μm) in millimetre-scale volumes in ~ 10 nanoseconds. At peak power, it generates up to 750 trillion Watts of laser light and is useful for both direct and indirect-drive experiments. It is claimed that with the full NIF, it would be possible to produce radiation dominated shocks similar to that occurring in the secondary of a thermonuclear device. Some laser facilities are listed below (Table-IV).

Table-IV: Main Laser facilities for HED Physics

Country	Laser	No. of Beams	Energy (kJ)	Pulse (ns)	λ (μm)
USA	NOVA	10	50	1	0.35
	NIF	192	1800	15	0.35
France	Megajoule	288	1800	15	0.35
Japan	KOYO	400	4000	6	0.35
Russia	ISKRA-5	12	15	0.25	1.3

Z-pinch Devices: In a typical Z-pinch device, a current pulse through a plasma column compresses and heats the plasma to temperatures in range of 10-100 eV. However, MHD instabilities set limits for confinement of plasma. Cylindrical liners and wire arrays for X-ray sources are also based on the pinch effect. It is now claimed that even 15 MJ of X-rays can be delivered to a dynamic hohlraum for indirectly driven fusion.

Ion beams: HED conditions can be realised on stopping high-velocity ions in a material like Pb. The two challenges with ion beams are: generation of short-time (ns) pulses; and deposition of energy in a small volume. Because heavier ions have larger positive charges, they can be stopped more rapidly over a given distance than lighter ions.

V. Basic Physics & Modelling

The fundamental physical phenomena that govern the physics of HED systems are listed in Table-V. Brief descriptions of these phenomena and typical results from our efforts in modelling and simulations will be discussed next.

Table-V: Physical Phenomena involved in HEDP	
Hydrodynamics & Shock Waves	Radiation driven Hydrodynamics
High Pressure EOS of Matter	Neutronics of Fission & Fusion Devices
Radiation Diffusion & Transport	Thermonuclear Ignition & Burn
Radiation Opacity of Plasmas	Hydrodynamic Instabilities

1. Hydrodynamics and Shock Waves:

Atoms or molecules acquire kinetic energy on receiving energy from an external source. This leads to formation of pressure gradients in the medium. Consequently, macroscopic motion, changes in density, internal energy, etc., can occur. Hydrodynamic processes may be initiated due to impact phenomena, explosive burn, lasers, ion beams or pulsed currents. It is described in terms partial differential equations in space-time for conservation of mass, momentum and energy. An equation of state giving pressure and internal energy, in terms of density and temperature, closes the set of equations. At lower pressures, material properties like yield stress, shear stress and plastic flow models are also required. Shock waves are formed when large amplitude hydrodynamic disturbances occur. Shock waves are sharp discontinuities in the fluid variables and propagate with a speed characteristic of the pressure. The medium behind the shock front is compressed and heated, the extent of which again depends on pressure behind the shock.

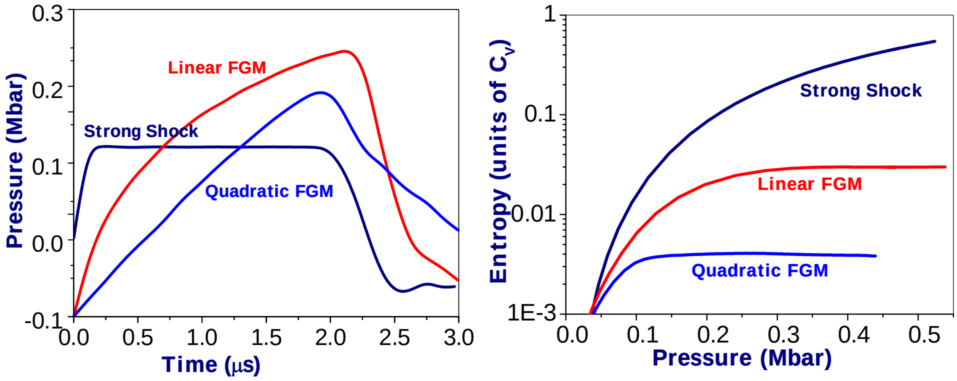

Fig. 4: Pressure and entropy variation in quasi-isentropic compression.

ICF invariably employs dynamic compression using shock waves because the fusion rate is proportional to square of pellet density. Though static compression using diamond anvil cell is useful for laboratory studies, it is inadequate for ICF. Dynamic schemes in nanosecond scales, via strong shocks are also not useful due to strong pre-heating of the medium. For example, strong shock can increase density in monatomic ideal gas only by 4 times. But, high compression is achievable using isentropic and quasi-isentropic methods, which occur over longer (microsecond) time scales (see Fig. 4). The ramp pressure pulse produces compression of the medium at low entropy. Lasers and magnetic fields are used to generate quasi-isentropic compression. Functionally graded materials (FGM) are now being used as impacting materials in gas guns or explosive driven systems [3, 4].

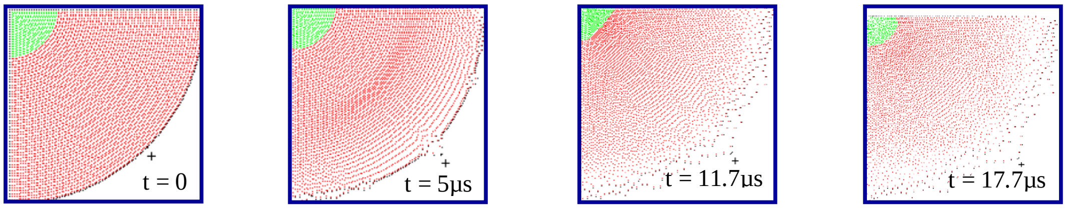

Fig.5: SPH simulation of explosive driven Aluminum sphere

Hydrodynamics simulations need efficient and robust algorithms [5, 6]. Mesh distorsions inherent in 2D and 3D Lagrangian schemes, have to be tackled with Eulerian, ALE (arbitrary Lagrangian-Eulerian) and the mesh free Smooth Particle Hydrodynamics (SPH) schemes. In SPH, each material is modelled as a collection of large number of interacting particles obeying the Eulerian conservation equations. Fig. 5 shows SPH simulation of different stages of implosion of a sphere by an explosive driven shock.

2. Equation of State:

Detailed knowledge of equation of state (EOS) is necessary for hydrodynamic simulations of matter. Tables of EOS over large range of density (10^{-4} to 10^{4} of normal density) and temperatures up to about 10^{9} K are needed for elements, compounds and alloys. Fig. 6 shows typical pressure isotherms of Be and energy isotherms of UH_3 up to 1 keV. We have developed extensive tables for a variety of materials, which are relevant to ICF and similar HED systems [7, 8].

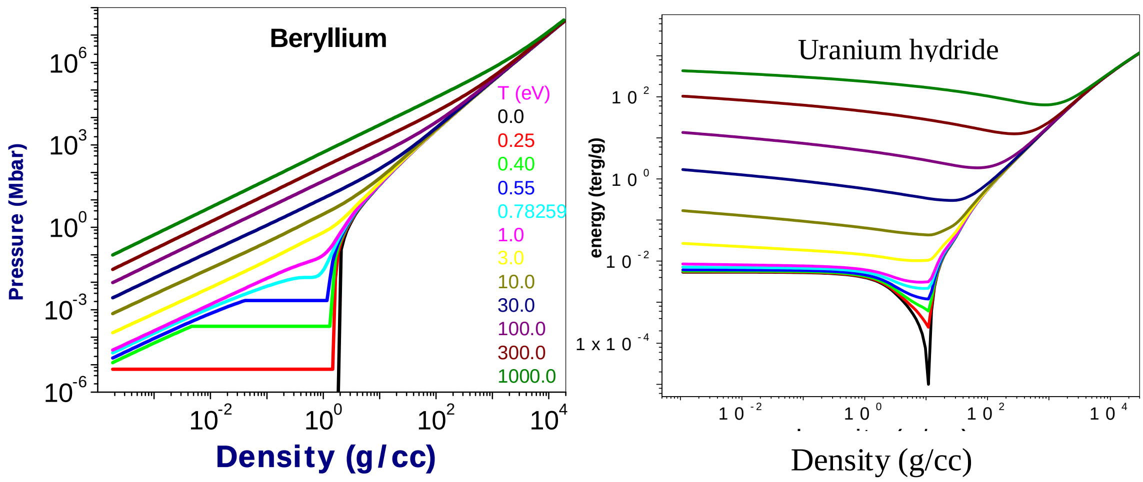

Fig. 6: Pressure isotherms of Be & Energy isotherm of UH_3

The EOS models must also account for the properties of materials in the expansion phase, i.e. for densities lower than those corresponding to their respective solid phases. Materials generally undergo the liquid-vapor phase transition and it is essential to have good predictions of EOS in this region. Accuracy of the EOS models can be checked against data obtained from shock release experiments. Fig. 7 shows comparisons from our EOS models for Hg near the critical point and Mo in release experiments [9].

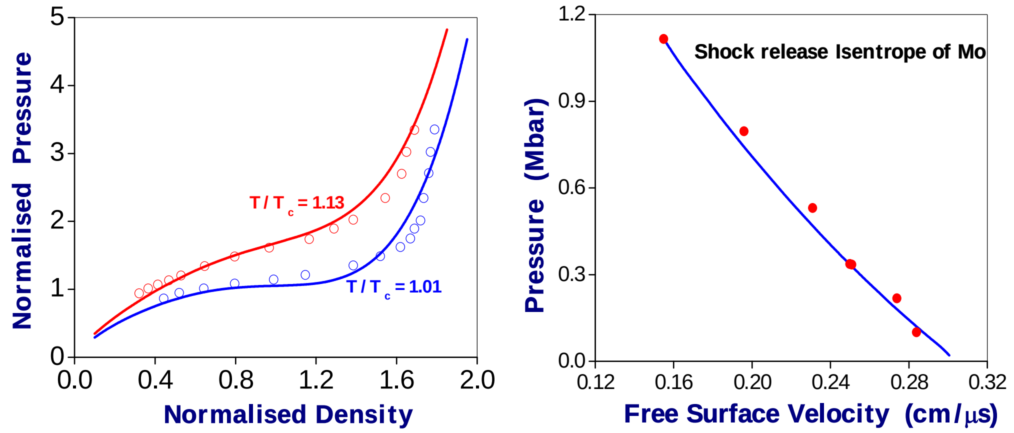

Fig. 7: EOS in liquid-vapour region – Critical point and Shock release

The problem of predicting the liquid-vapor phase diagram in the region close to critical point needs correct accounting of fluctuations using renormalization group theories [10]. However, away from the critical point, an accurate statistical mechanical calculation of free energies, using perturbation theories, is needed [11]. Further, it is necessary to use appropriate potentials like the embedded atom method (EAM) potential for metals [12]

Materials undergo different types of phase transitions during shock wave propagation. Structural phase transitions, melting, vaporization, etc. are possible phase changes. Correct modelling of atomic motion and structural aspects are needed to predict these transitions as they occur due to small changes in energy and/or entropy. We use models based on solid state theories [13-15] and liquid state theories [16-17], which incorporate, among other features, an-harmonic atomic vibrations. Fig. 8 shows results for shock induced α-ε transition in Fe and melting curve for Al.

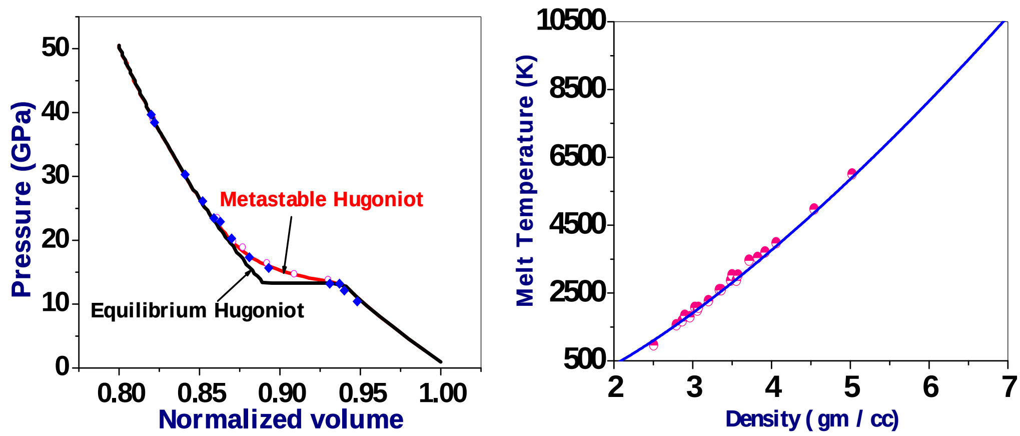

Fig. 8: Shock induced phase transition in Fe and melting of Al

Electronic excitation induced by shock and subsequent heating is the main contribution to EOS at high pressures. When a solid is compressed along the zero temperature isotherm (theoretically), electrons are ionized due to pressure ionization, which has origin in Pauli's exclusion principle. Our recent calculations (see Fig. 9) for Be and Li, based on Englert and Schwinger model are in excellent agreement with the TFDW model. This model includes effects of electron exchange and quantum corrections to semi classical theory [18,19].

Heating of materials by shocks also leads to thermal ionization. This manifests as oscillations in the high pressure Hugoniot plots. Predictions from our model and comparison with data for Al up to 10^4 Mbar are also shown in this figure [20]. We have also include radiation pressure, which exceeds material pressure around 5 keV. This model also was used to study the effect of ionization on the stability of shock waves [21].

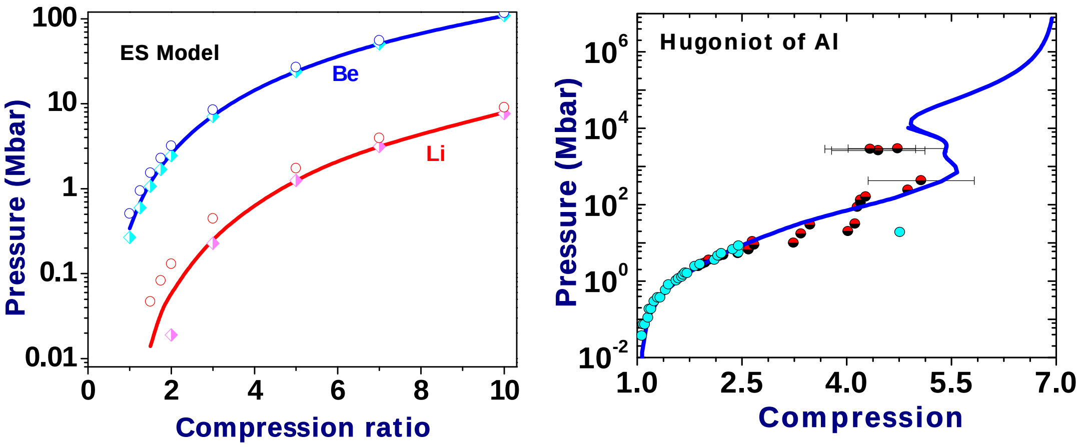

Fig. 9: Electron and radiation contributions to EOS

3. Radiation Opacity:

Radiation transport in HED matter requires frequency dependent absorption and emission coefficients, usually known as opacities. Because of changes in electronic structure due to pressure and thermal ionization, opacity depends on density, temperature and compositions of the materials.

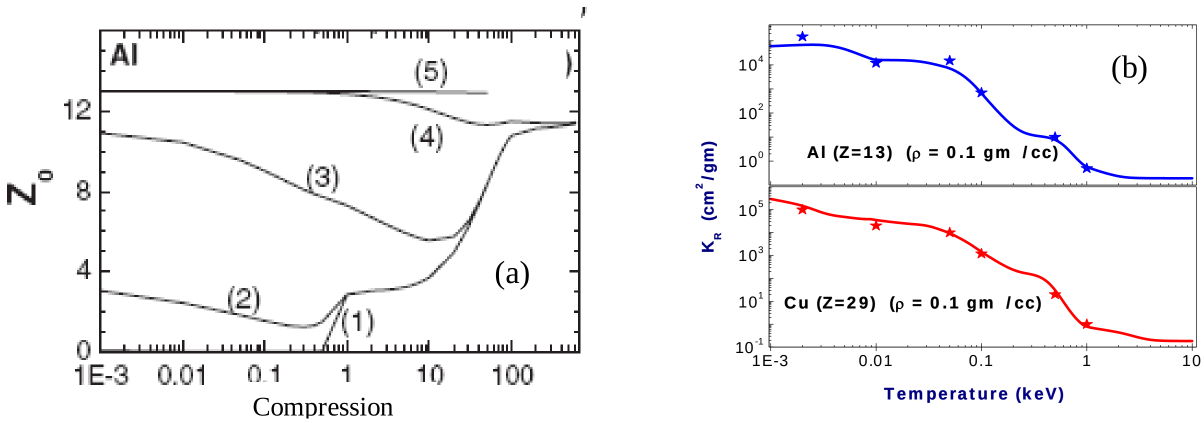

Fig. 10: Ionization in Al and opacity of Al, Cu

Variations of ionization in Al with compression at temperatures 0.001, 0.01, 0.1, 1 and 6 keV are shown in Fig 10(a) [22]. Pressure ionization is evident in this figure for low temperatures such as 0.001 & 0.01 keV. Investigations of pressure ionization and radiation opacities in hydrogen like plasmas, using bound and continuum energies and wave functions obtained from solution of Schrodinger equation, have also been done [23].

Extensive tables for radiation opacity are needed for simulations. These have to be computed using detailed atomic structure methods, since measurements of in the entire range of parameters are impossible. Atomic theory should also include, among other details, the effects plasma environment on electron energy levels. The concept of local thermodynamic equilibrium can be used for calculating opacities in dense matter. However, non-equilibrium effects are quite important in dilute plasmas produced by ablation. Typical results for the temperature dependent Roseland opacities [22] of Al and Cu are shown in Fig. 10(b).

4. Radiation Transport:

Evolution of thermal X-rays in hohlraum, which is a cavity made with a high-Z material, is an important problem in indirect-drive fusion. The intensity of X-rays falling on fusion capsule and its angular uniformity determine the adequacy of the hohlraum. Modelling this problem needs multidimensional radiation transport. Fig. 11 shows peak temperatures obtained in a gold hohlraum for different laser powers. The temporal evolution of radiation temperature, for a particular laser pulse, is also shown on in the figure [24, 25]. Inset in the latter figure is the time history of input laser power.

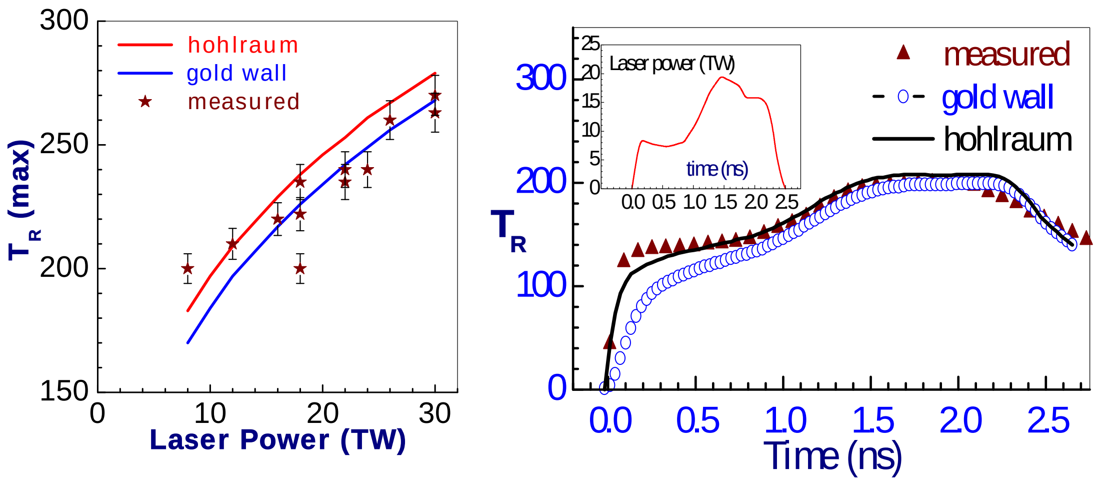

Fig. 11: Evolution of radiation temperature in hohlraum

Important aspects of simulating the hohlraum are absorption and re-emission of X-rays from the walls, leakages via openings and hydrodynamics of wall. In additions to radiation transport theory (based on discrete ordinates methods), we have also developed diffusion and view factor methods. The latter ones are suitable for nearly isotropic X-ray distributions [26].

5. Radiation Hydrodynamics:

Modelling radiation driven hydrodynamics is an essential ingredient for HEDP. In these problems, radiation transport equation in a moving medium, is solved together with hydrodynamics equations in a self-consistent manner. Fig. 12(a) displays position of the radiation shock generated in an Al foil when a X-ray pulse (see Fig. 11(b)) is incident on it. There are two distinct slopes and hence two shock speeds corresponding to two plateaus in the incident profile. Fig. 12(b) shows the profiles of the scaled thermodynamic variables in the radiation driven shock in a point explosion problem [27].

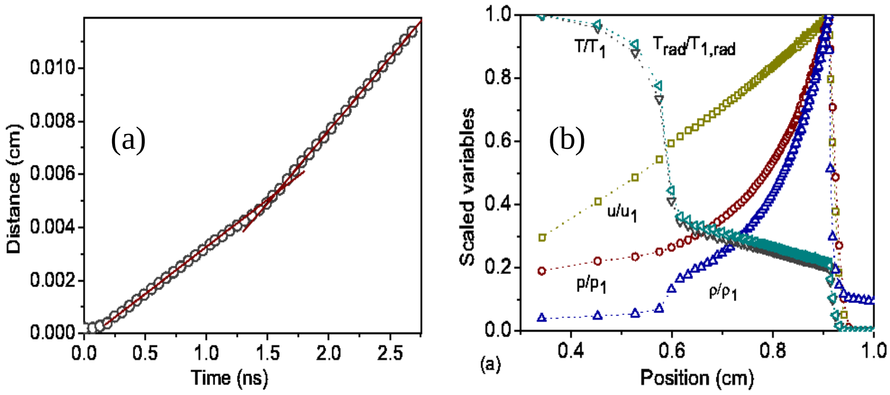

Fig. 12: Radiation driven hydrodynamics and shock waves

6. *Thermonuclear Burn:*

Most of the ICF schemes employ the concept of central ignition wherein only a central hot spot of the capsule is heated to few keV while the remaining fuel is only compressed to high densities. For a specified temperature of the hot spot, there is a critical value of the areal density (product of mass density and its radius) for sustained burning of fuel.

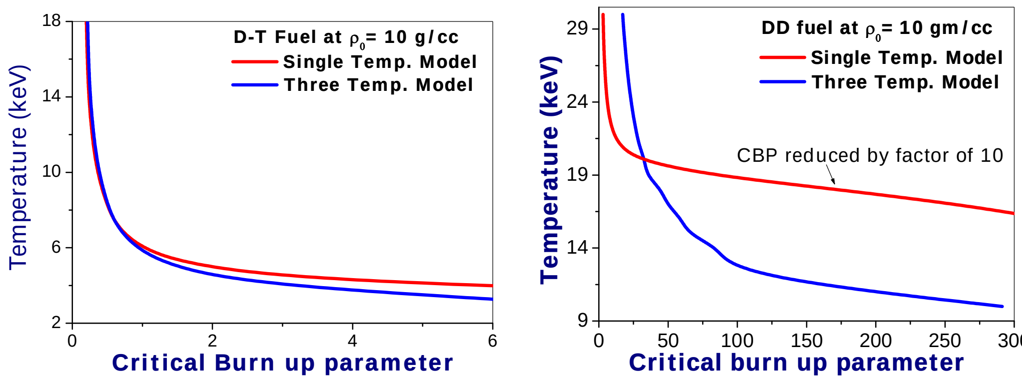

Fig. 13: Critical hot spot parameters for thermonuclear burn

We have developed a three-temperature model (ion, electron and radiation) to estimate this critical parameter for different types of fusion fuels [28]. Fig. 13 shows that for D-T fusion a single temperature model is adequate while for D-D fusion non-equilibrium effects are quite important. This is due to lower fusion cross-sections for the latter.

7. *Tritium Breeding:*

It is interesting to explore the possibility of tritium breeding together with the fusion reactions. We developed a model that includes nuclear scattering and large angle Coulomb scattering of charged particles and collective plasma effects. All the radiative loss mechanisms like the bremsstrahlung, inverse Compton scattering and photon leakage from pellet are also added. Fig. 14(a) shows energy leakage probability of D ions against pellet radius in a deuterium plasma. Three cases of energy loss are shown: (i) only to electrons, (ii) electrons and ions and (iii) also including nuclear scattering. Fig. 14(b) shows tritium, normalised to its initial amount, left in the pellet at different times when various energy exchange mechanisms are included. While curve (i) is for bremsstrahlung loss only, curve (ii) also including inverse bremsstrahlung. For curve (iii), inverse Compton scattering is also considered. These results indicate the importance of the various mechanisms needed to be included [29, 30].

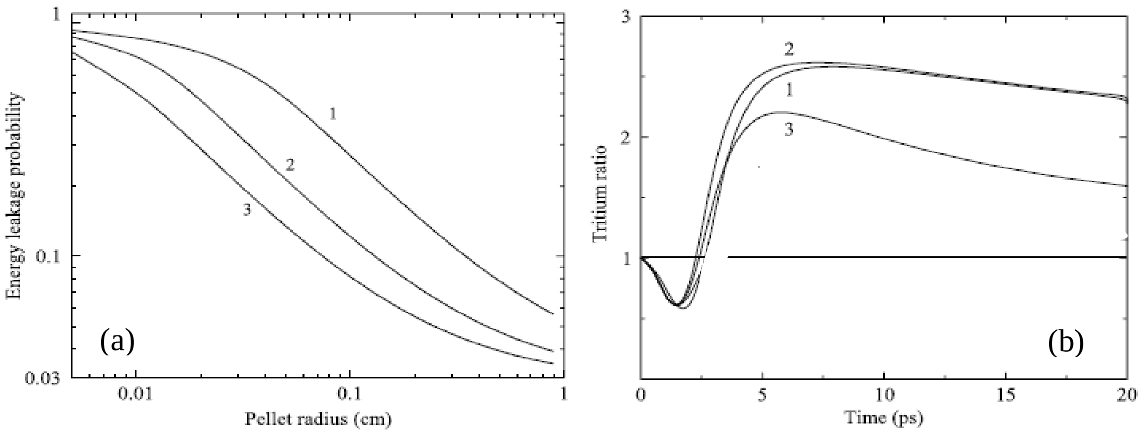

Fig. 14: Energy leakage of probability of D_2 in Fusion Plasma and Tritium Breeding

8. Particle transport theory:

Energy deposition in ICF pellet by neutrons and charged particles is to be accounted in the simulations. In fact, this is what sustains burning of the fuel. Particle transport theory can be used for these calculations if compilations of interaction cross-sections of particles with various materials are available. These data are generally converted to cross-section libraries. Details of these aspects of simulations shall not be covered in this article.

Another application of transport theory, involving neutrons, γ-rays and electrons, is in modelling the generation and propagation of the nuclear electromagnetic pulse (NEMP) from a nuclear event [31-33].

9. Hydrodynamic instabilities:

An ideal implosion of ICF capsule should have perfect spherical symmetry. However, this does not occur due to inherent growth of hydrodynamic instabilities during the implosion. Nonuniform irradiation, roughness of capsule surface and deviations from perfect sphericity of shells are some of the causes of instabilities. Rayleigh-Taylor instability arises when lighter ablated plasma is accelerated into denser un-ablated mass. Richtmayer-Meshkov instability occurs when a shock wave crosses an interface between two media of unequal density. Determining the effect of these instabilities is a daunting task as it needs numerical schemes of high precision and accuracy.

VI Conclusions

This article discussed some of the important aspects of HED systems. Our main emphasis has been on the pheneomena involved in ICF, eventhough similar physics occur in other applications that we have mentioned. Brief outlines of the different topics involved are discussed together with some of our own results in these areas.

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