

Agenda for APEX-6/FHPD Workshop
University Of California-Los Angeles
February 16-19, 1999
Faculty Center/James West Center

*Numerical Simulation of Melting and Evaporation
Due to Ultra-Short-Pulse Laser Irradiation*

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Objectives

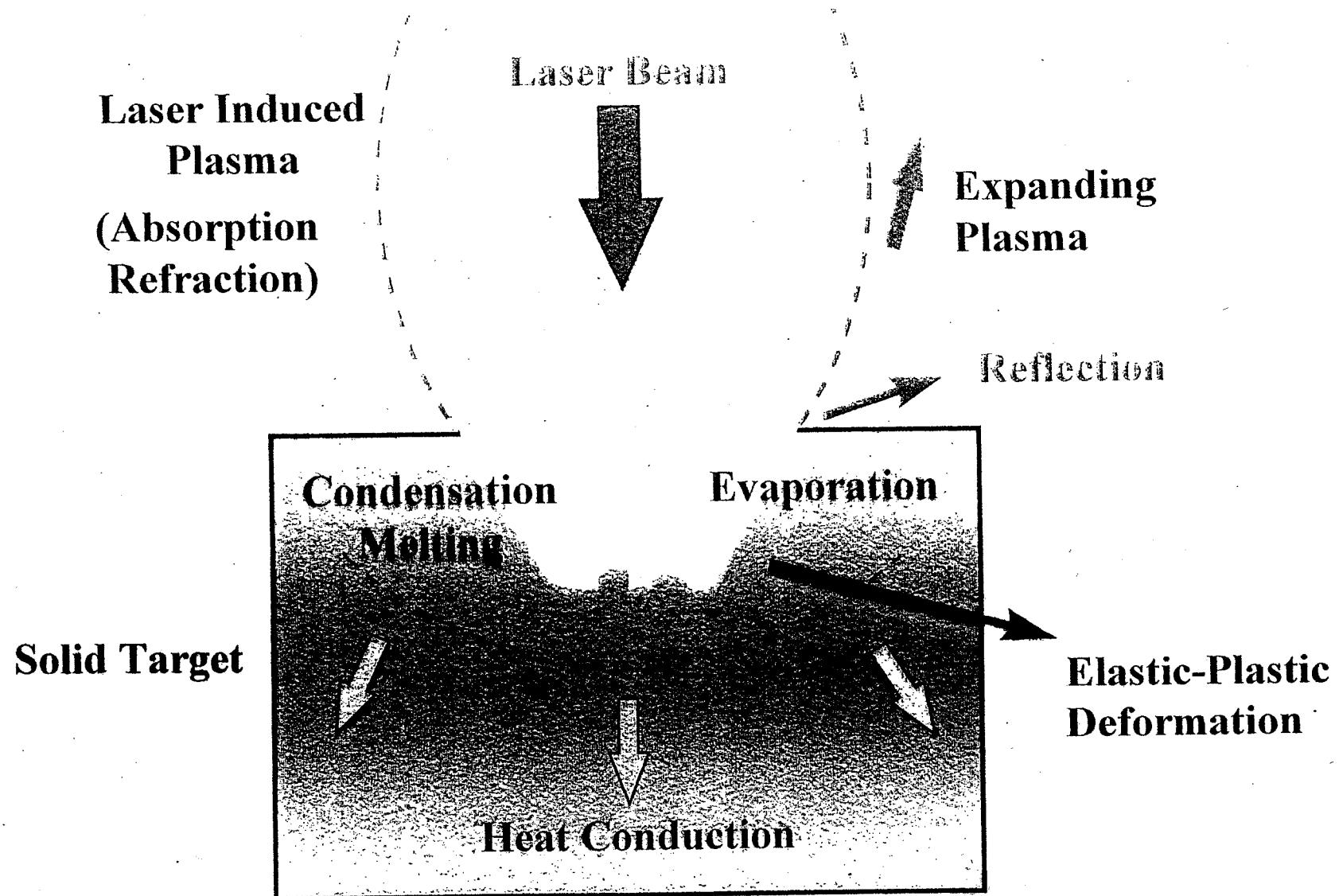
- (1) To develop a hydrodynamic code based on a robust scheme ;**

CIP (Cubic-Interpolated Propagation)

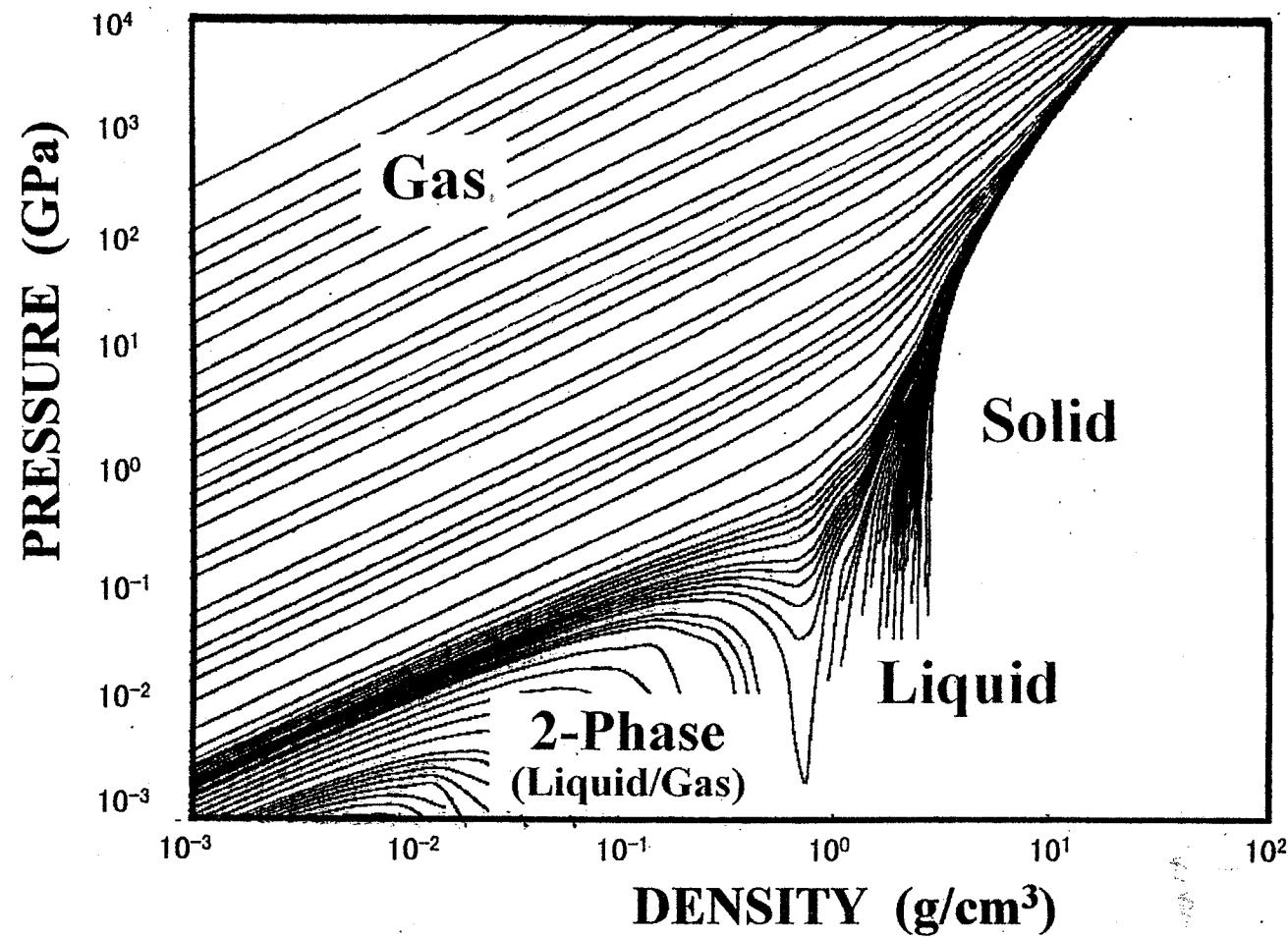
C-CUP (CIP-Combined Unified Procedure)

- (2) To demonstrate the potentiality of the code for laser-induced melting and evaporation**

Hydrodynamics of Laser-Matter Interaction



SESAME EOS DATA(ALUMINUM)



Difficulties in Simulation of Melting and Evaporation

1) Density Difference

Metal $1 \sim 10 \text{ g/cm}^3$

Air $\sim 10^{-3} \text{ g/cm}^3$

2) Phase Change

Co-existing 3 phase : solid-liquid-gas

$\delta\rho \sim 10\% \Rightarrow \delta P \sim 10^{3\sim 4}$

C_s : Solid (Al) $\sim 5 \times 10^3 \text{ m/s}$

Air $\sim 3 \times 10^2 \text{ m/s}$

3) Surface Deformation

Outline of a Hydrodynamic Code

(1) Cartesian Coordinate : $x-y-z$

(2) Staggered Grid Arrangement

•Scalar (P, ρ) : Cell Center

•Vector(u, v, w) : Cell Interface

(3) Computational Algorithm

•CIP Method (Cubic Interpolated Propagation)

•C-CUP Method (CIP-Combined Unified Procedure)

•Interface Function (ϕ)

(4) EOS Including 3 Phases, Solid, Liquid and Gas ($P-\rho-T$)

Governing Equations

(Mass)
$$\frac{\partial \rho}{\partial t} + \vec{u} \cdot \nabla \rho = -\rho \cdot \operatorname{div} \vec{u} \quad (1)$$

(Momentum)
$$\frac{\partial \vec{u}}{\partial t} + \vec{u} \cdot \nabla \vec{u} = -\frac{1}{\rho} \nabla p + \nu \cdot \Delta \vec{u} + \vec{F}_{sa} + \vec{g} \quad (2)$$

(Energy)
$$\frac{\partial \varepsilon}{\partial t} + \vec{u} \cdot \nabla \varepsilon = -\frac{p}{\rho} \operatorname{div} \vec{u} + \frac{\lambda}{\rho} \cdot \Delta T + \frac{Q}{\rho} \quad (3)$$

(Interface)
$$\frac{\partial \phi_i}{\partial t} + \vec{u} \cdot \nabla \phi_i = 0 \quad (4)$$

(EOS)
$$\varepsilon = f(\rho_i, T) \quad \rho = \sum_i \rho_i \phi_i \quad \rho \varepsilon = \sum_i \rho_i \varepsilon_i \quad (5)$$

$$p = f(\rho_i, T) \quad \sum_i \phi_i = 1$$

CIP Method

• Fractional step :

Splitting hyperbolic eqs. into two steps, advection and non-advection phases.

$$\frac{\partial f}{\partial t} + \vec{u} \cdot \nabla f = g \quad (\text{Hyperbolic eqs.})$$

Advection

$$\frac{\partial f}{\partial t} + \vec{u} \cdot \nabla f = 0$$

Explicit differencing scheme with a cubic polynomial ;

$$F=F(f, f_x, x)$$

Non-advection

$$\frac{\partial f}{\partial t} = g$$

Implicit differencing scheme

C-Cup Method

- Non-advection phase

Implicit differencing of Poisson-like eq. from momentum and p based energy eqs.

$$\left(\sum_i \rho_i \phi_i \left(\frac{\partial \varepsilon_i}{\partial p} \right) \right) \frac{Dp}{Dt} = \left(\sum_i \rho_i^2 \phi_i \left(\frac{\partial \varepsilon_i}{\partial \rho_i} \right) - p \right) \cdot \operatorname{div} \vec{u} + \operatorname{div}(\lambda \cdot \operatorname{grad} T) + Q$$



↑
Substituting $\frac{\partial \vec{u}}{\partial t} = -\frac{1}{\rho} \nabla p$

$$\left(\sum_i \rho_i \phi_i \left(\frac{\partial \varepsilon_i}{\partial p} \right) \right) \frac{Dp}{Dt} = \left(\sum_i \rho_i^2 \phi_i \left(\frac{\partial \varepsilon_i}{\partial \rho_i} \right) - p \right) \cdot \operatorname{div} \left(-\frac{\Delta t \cdot \operatorname{grad} p}{\rho} + \vec{u}^n \right) + \operatorname{div}(\lambda \cdot \operatorname{grad} T) + Q$$

Unified procedure is obtained for compressible and incompressible fluids.

Treatment of Energy Equations

The pressure p is treated as the dependent variable in place of internal energy ε in Eq.(3).

$$\left(\sum_i \rho_i \phi_i \left(\frac{\partial \varepsilon_i}{\partial p} \right) \right) \frac{Dp}{Dt} = \left(\sum_i \rho_i^2 \phi_i \left(\frac{\partial \varepsilon_i}{\partial \rho_i} \right) - p \right) \cdot \operatorname{div} \vec{u} + \operatorname{div} (\lambda \cdot \operatorname{grad} T) + Q$$

Gamma-Law Fluid

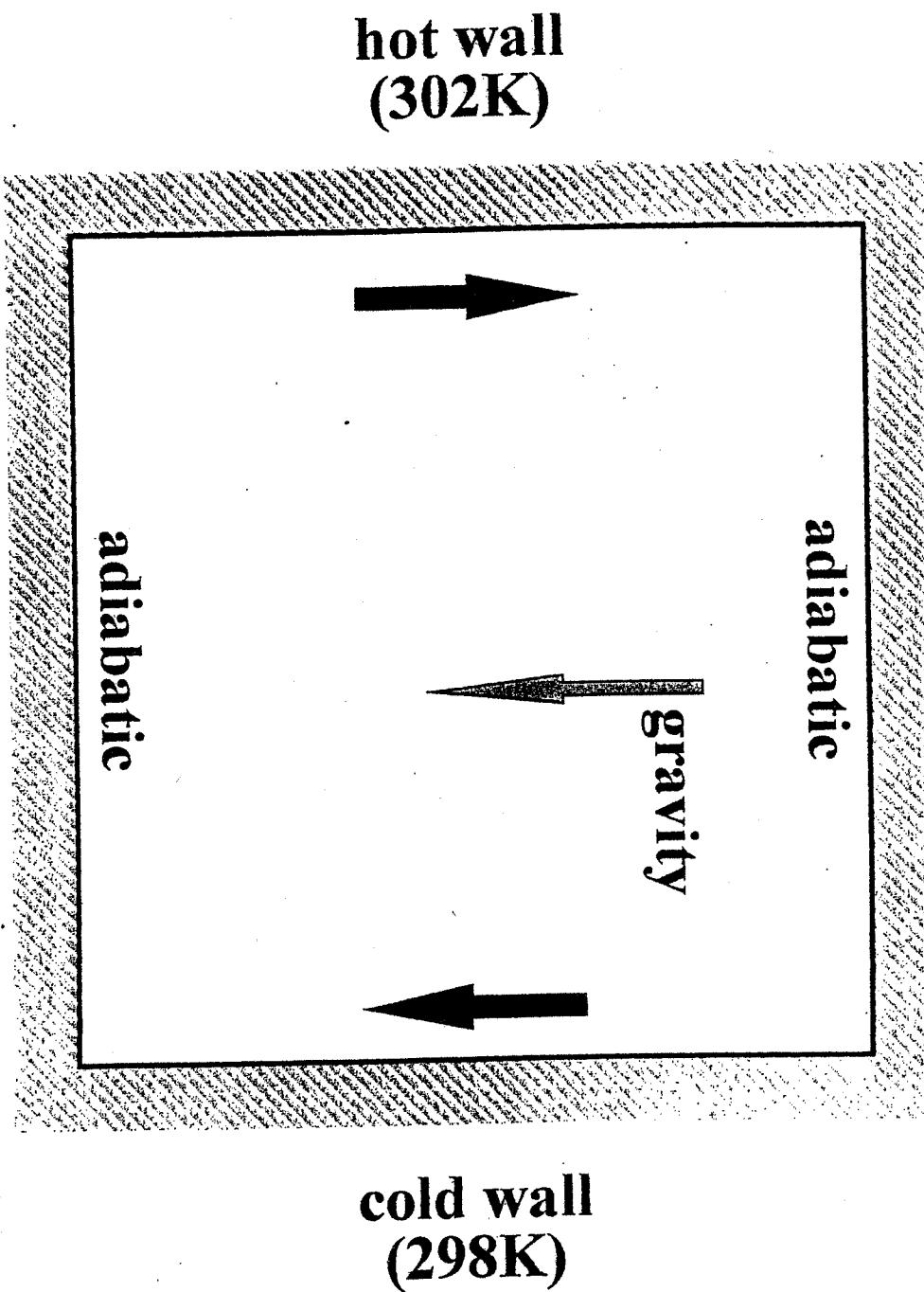
$$\frac{\partial \varepsilon}{\partial p} = \frac{1}{\gamma - 1} \cdot \frac{1}{\rho}, \quad \frac{\partial \varepsilon}{\partial \rho} = \frac{1}{\gamma - 1} \cdot \left(-\frac{p}{\rho^2} \right)$$

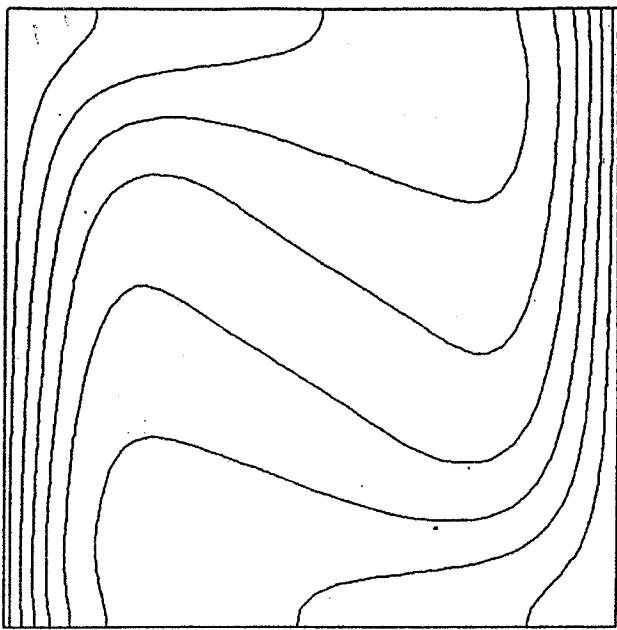
The above eqs. can be applied for multiphase and multicomponent flows.

Benchmark Problems

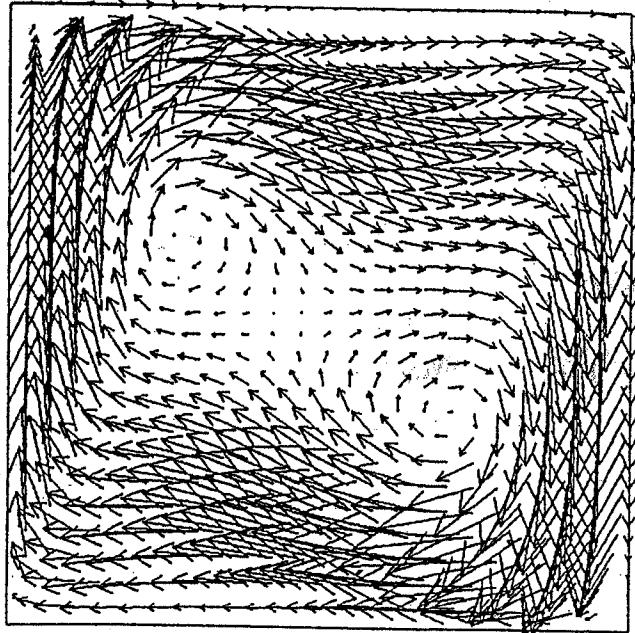
- (1) Natural Convection in a Square cavity**
- (2) Shock Tube with a Step**
- (3) Liquid Drop Deformation in a Shock Tube**

Natural Convection ($\text{Ra}=10^5$)

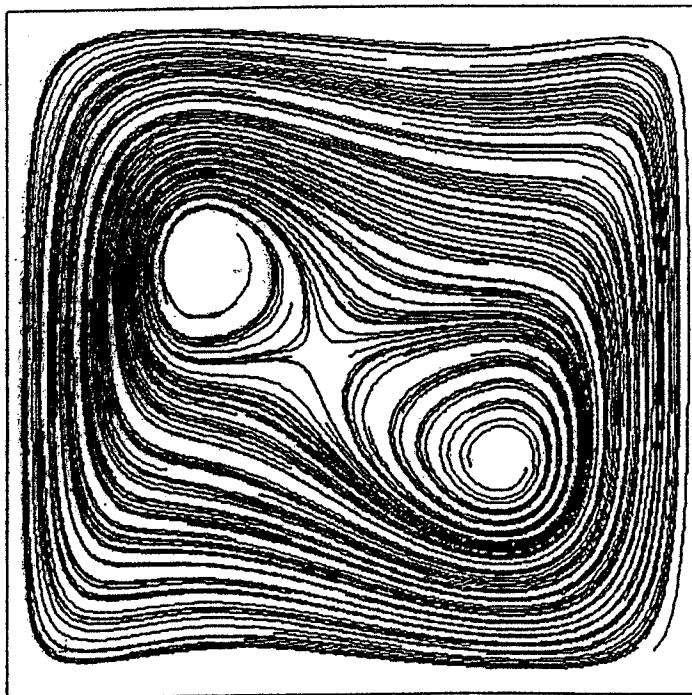




(a) 等温線分布

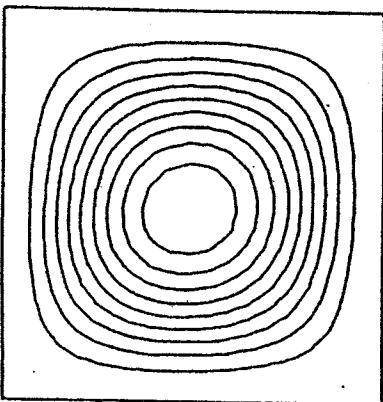


(b) 流速ベクトル

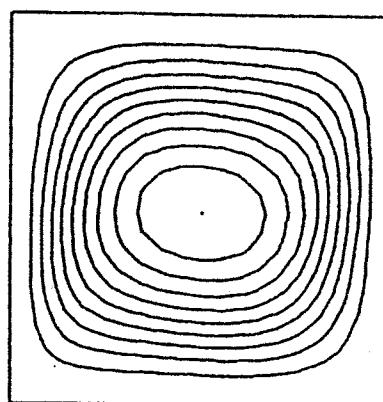


(c) ストリームライン

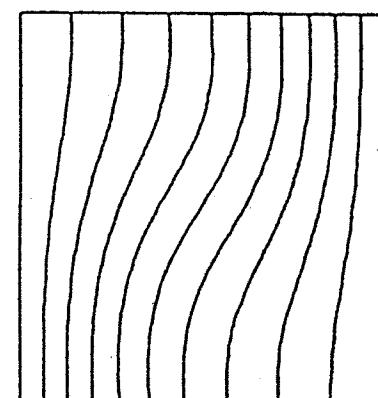
定常状態での矩形容器内の自然対流($\text{Ra}=10^5$, SESAME EOS ID=5761(He))



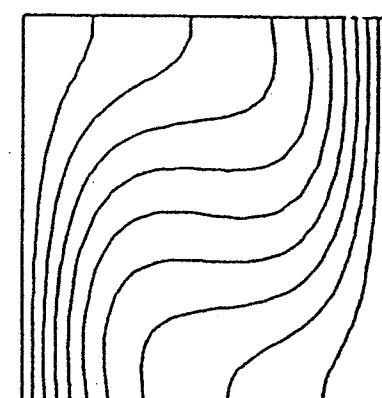
(a)



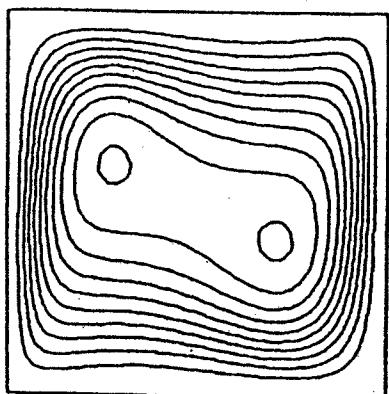
(b)



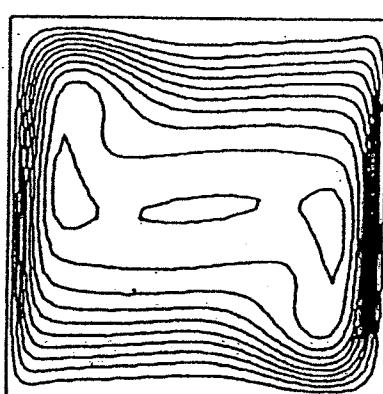
(a)



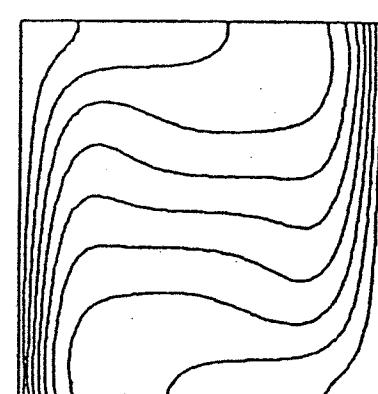
(b)



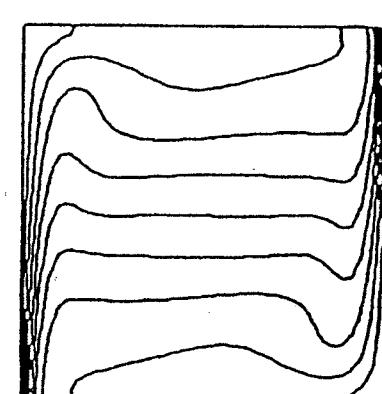
(c)



(d)



(c)



(d)

Figure 3. Contour maps of stream function ψ :

- (a) $Ra = 10^3$; contours at $-1 \cdot 174(0 \cdot 1174)0$;
- (b) $Ra = 10^4$; contours at $-5 \cdot 071(0 \cdot 5071)0$;
- (c) $Ra = 10^5$; contours at $-9 \cdot 507, -8 \cdot 646(0 \cdot 9607)0$;
- (d) $Ra = 10^6$; contours at $-16 \cdot 27, -15 \cdot 07(1 \cdot 675)0$

Figure 4. Contour maps of temperature T :

- (a) $Ra = 10^3$, (b) $Ra = 10^4$,
 - (c) $Ra = 10^5$, (d) $Ra = 10^6$.
- Contours at $0(0 \cdot 1)1$ in each case

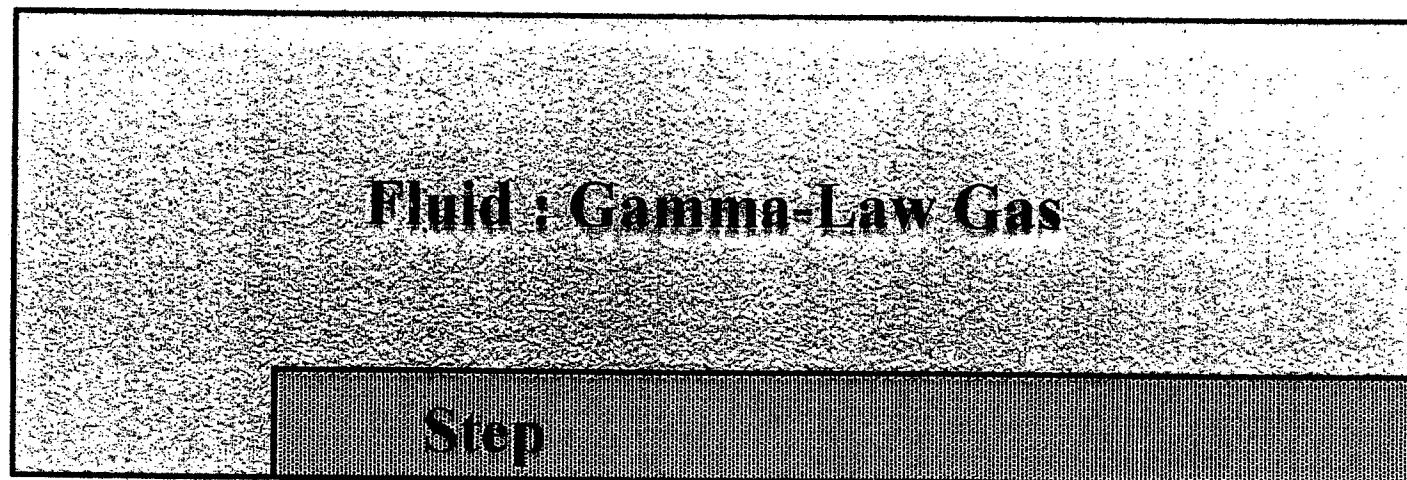
矩形容器内の自然対流例題計算

(De Vahl Davis, Natural Convection of Air in a Square Cavity, Int. J. Numerical Method in Fluids, Vol. 3, pp249-264(1983))

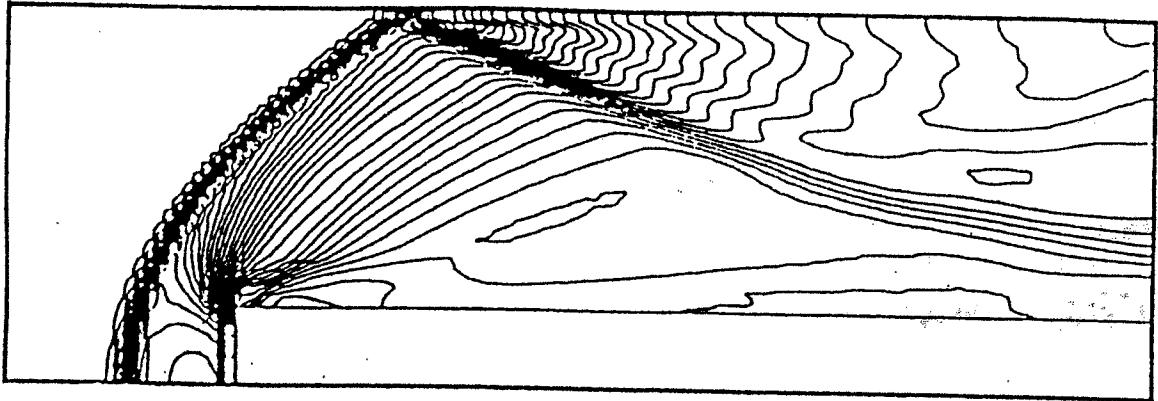
Shock Tube with a Step

Two-Dimensional Supersonic Flow
(Mach=3)

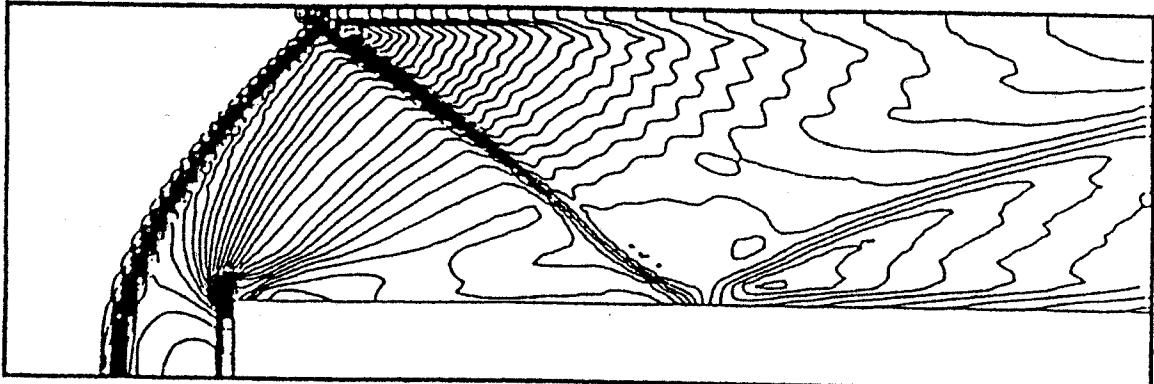
$u=3$
 $p=1$
 $\rho=1.4$



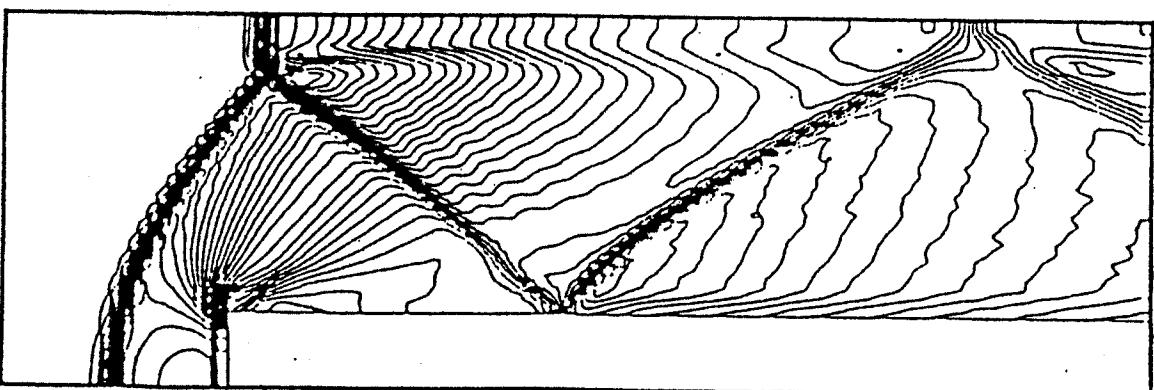
$t = 1$



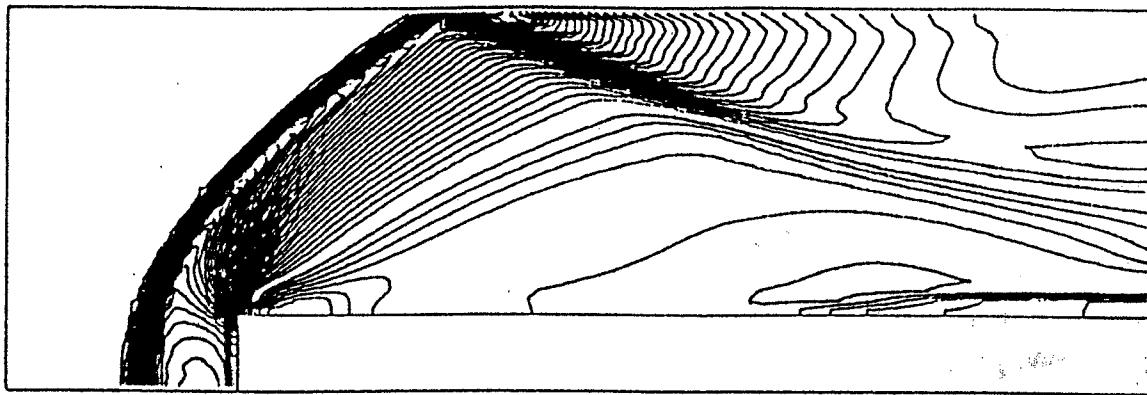
$t = 2$



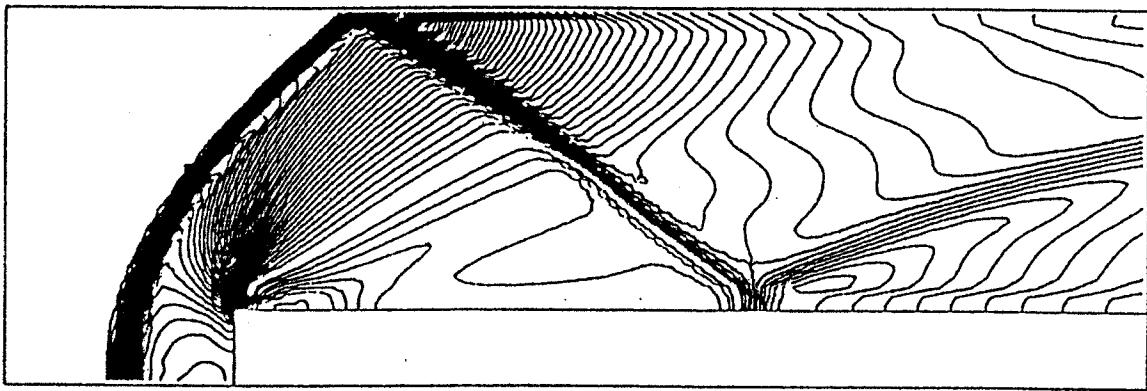
$t = 4$



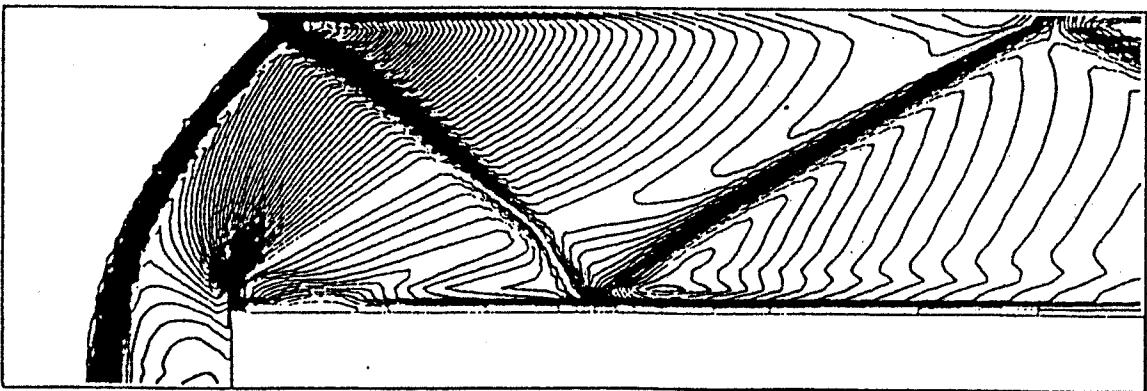
Yabe, Ishikawa and Wang



$t = 1$

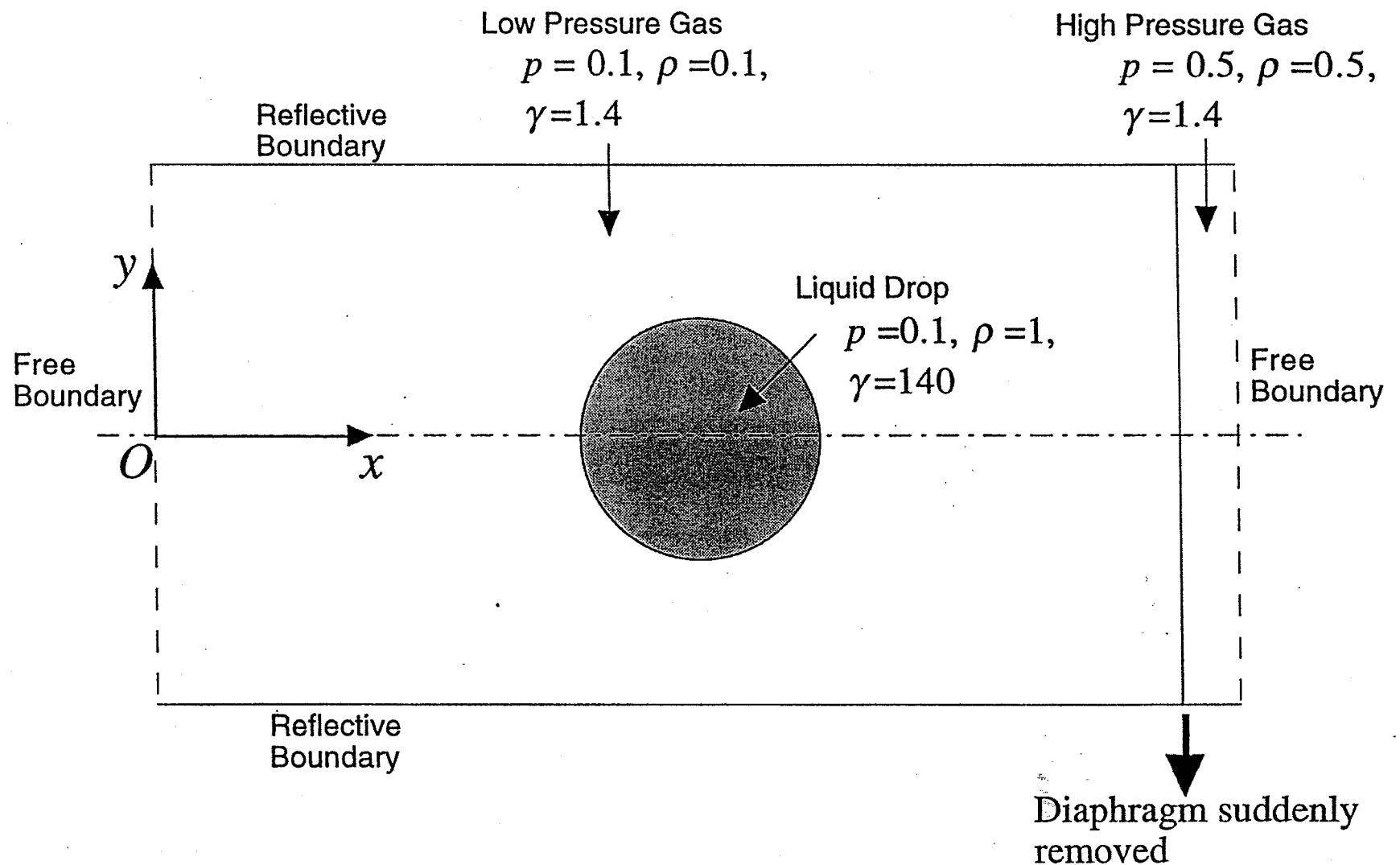


$t = 2$



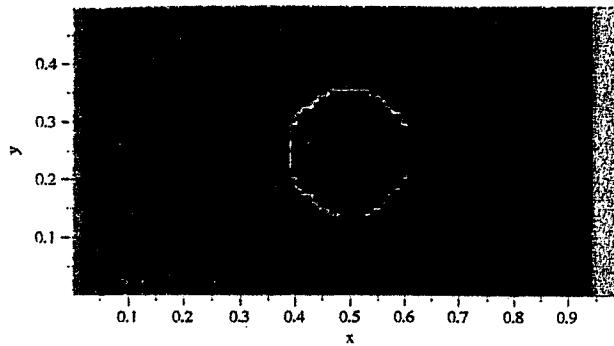
$t = 4$

Present calculation



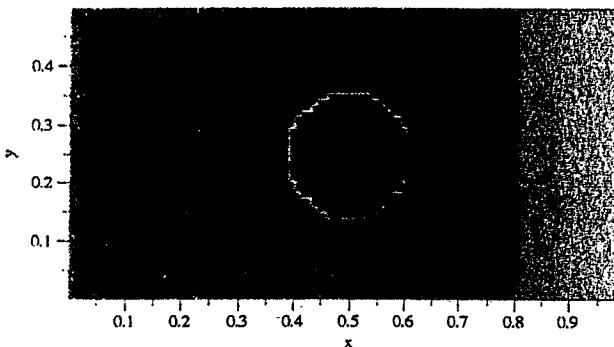
Ful90dtx.rhfx.GM140.f, 90x46, dt=5e-4(fixed) Cvis=0, Min-max filter used, Density at t=0.

t=0.0 (initial state)



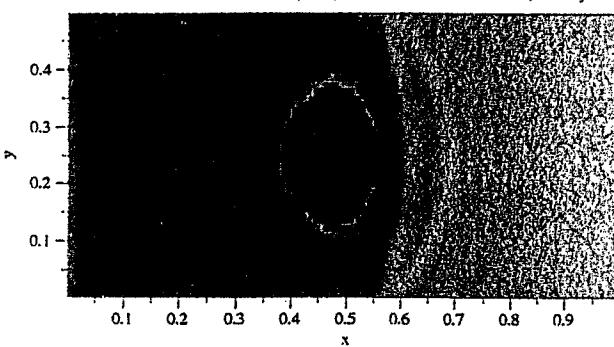
Ful90dtx.rhfx.GM140.f, 90x46, dt=5e-4(fixed) Cvis=0, Min-max filter used, Density at t=0.0625.

t=0.0625



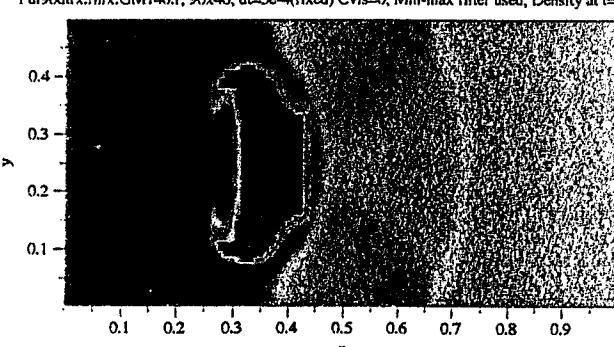
Ful90dtx.rhfx.GM140.f, 90x46, dt=5e-4(fixed) Cvis=0, Min-max filter used, Density at t=0.125.

t=0.125



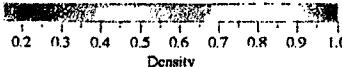
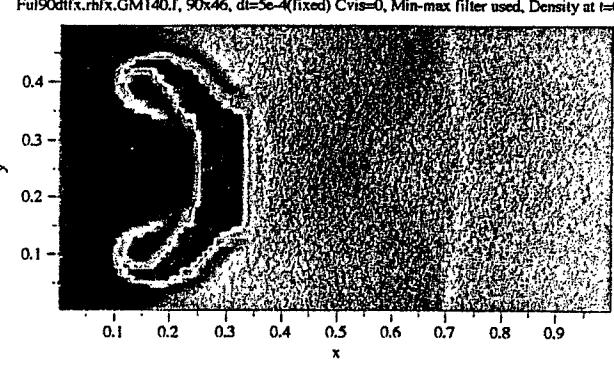
Ful90dtx.rhfx.GM140.f, 90x46, dt=5e-4(fixed) Cvis=0, Min-max filter used, Density at t=0.1875.

t=0.1875



Ful90dtx.rhfx.GM140.f, 90x46, dt=5e-4(fixed) Cvis=0, Min-max filter used, Density at t=0.225.

t=0.225

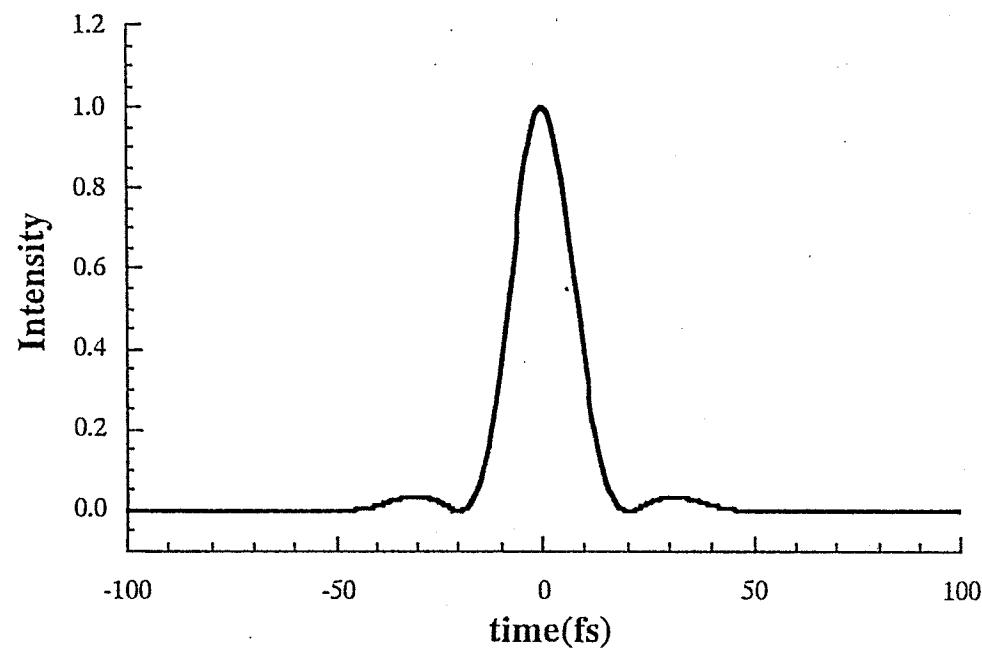


Liquid drop deformation in a shock tube. C-CUP with density function method.

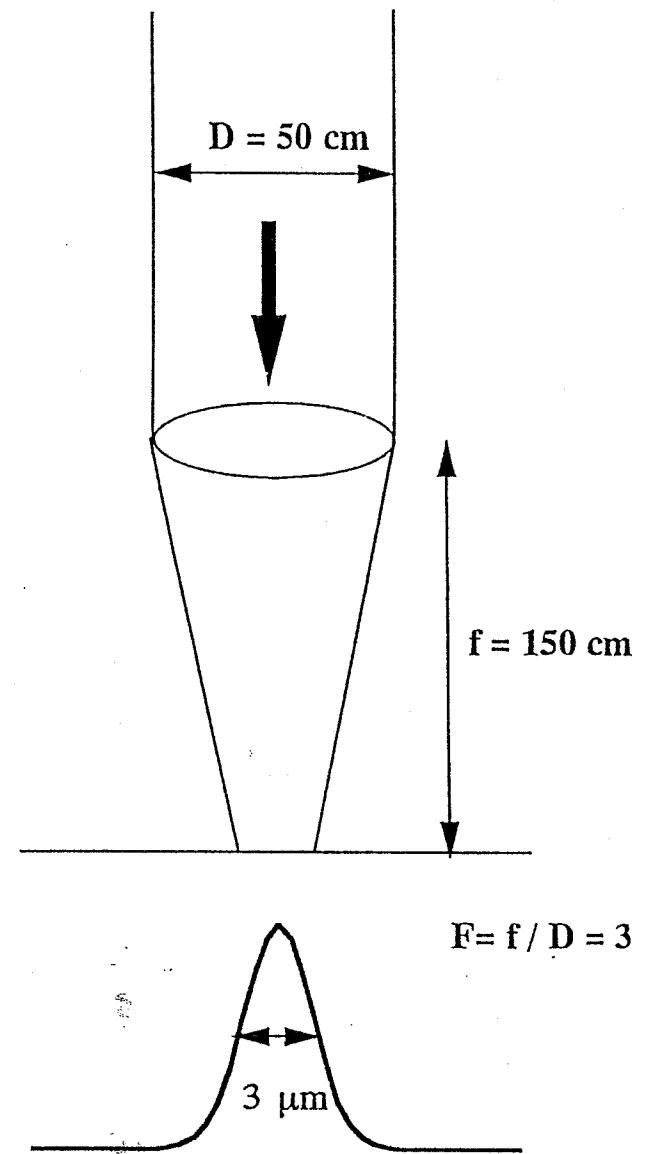
Laser characteristics

Peak Power 100TW

Wave Length 800nm



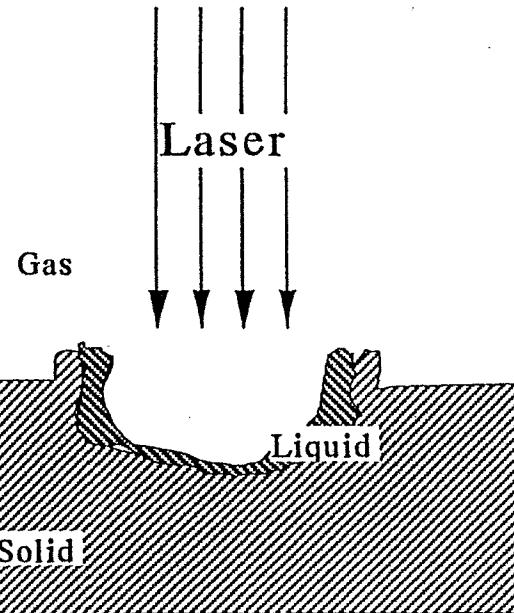
temporal profile



spatial profile

Phenomena

Solid • Liquid • Gas
(Multi-Phase,
Multi-Component,
Phase transition)



Model

Continuum equation

material properties

EOS(Equation of State)
transportation coeff.
electeical conductivity
thermal conductivity
absorption coeff.
skin depth

Laser characteristics

Numerical Method

Numerical Solver
based on
CIP and C-CUP scheme

CIP : Cubic Interpolated Propagation
C-CIP : CIP - Combined Unified Procedure

Computational System

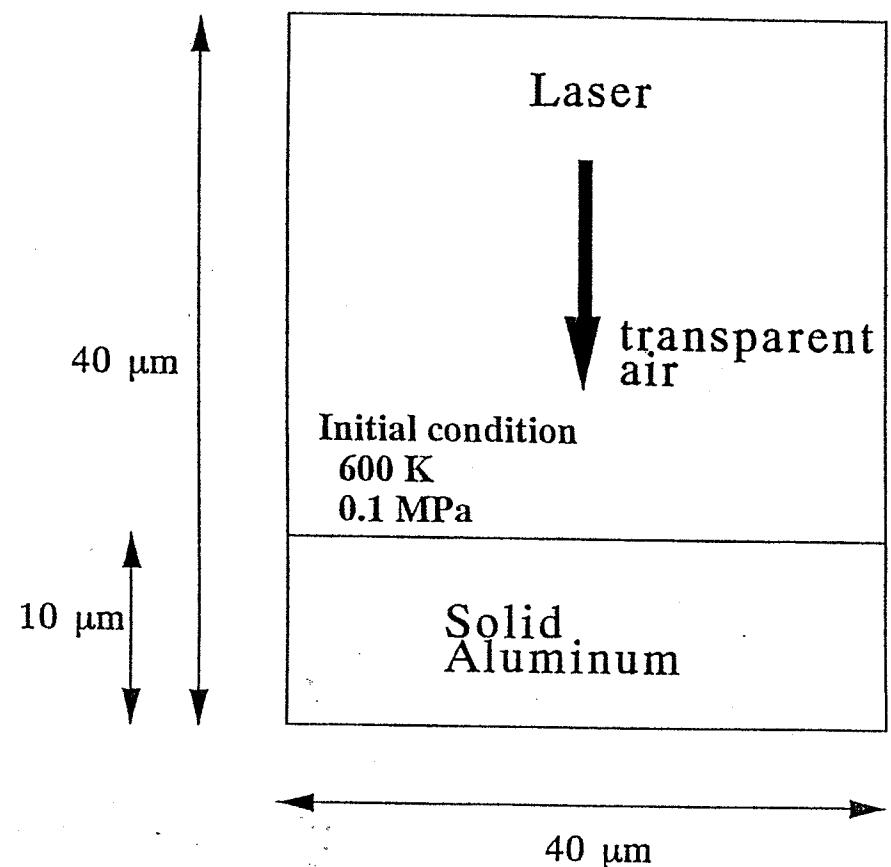
2 Dimension

Mesh No. 80×80

Mesh size $0.5 \times 0.5 \mu\text{m}$

Time step
 $0.25 \text{ fs (0 - 40 fs)}$
 $10 \text{ fs (40 fs - 1 ps)}$
 $100 \text{ fs (1 ps - 10 ps)}$
 $500 \text{ fs (10 ps - 500 ps)}$

CPU time $\doteq 3 \text{ Hr (DEC-alpha)}$

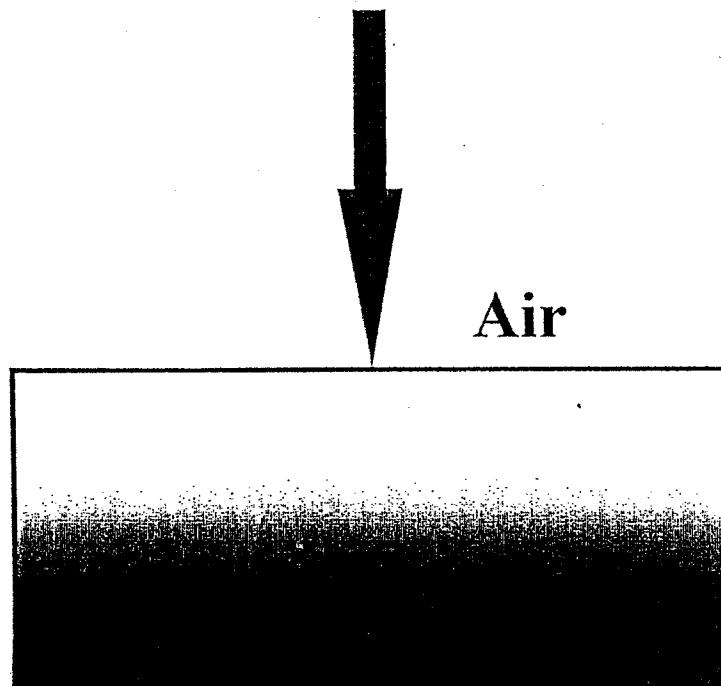


Numerical Simulation

Laser Beam

$Q : 10^{18} \text{ W/cm}^2$

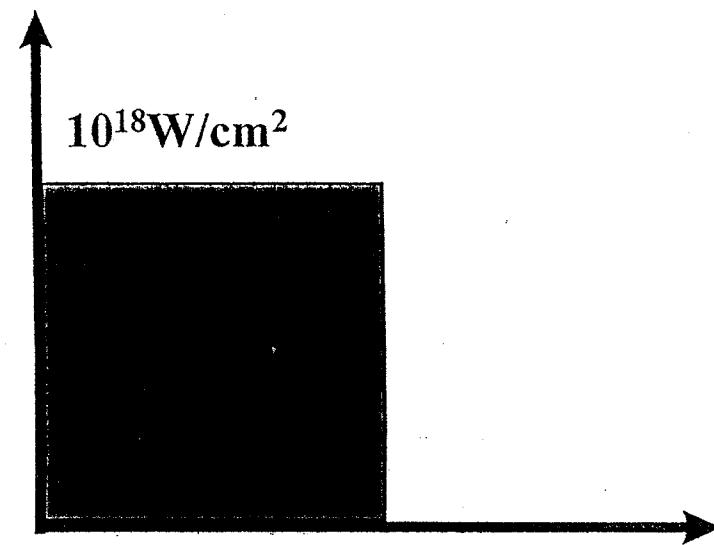
Spot Diameter : $10\mu\text{m}$



Intensity of Laser Pulse

10^{18}W/cm^2 , 30fs Pulse

Intensity



Aluminum

30fs

Time

Equation of State

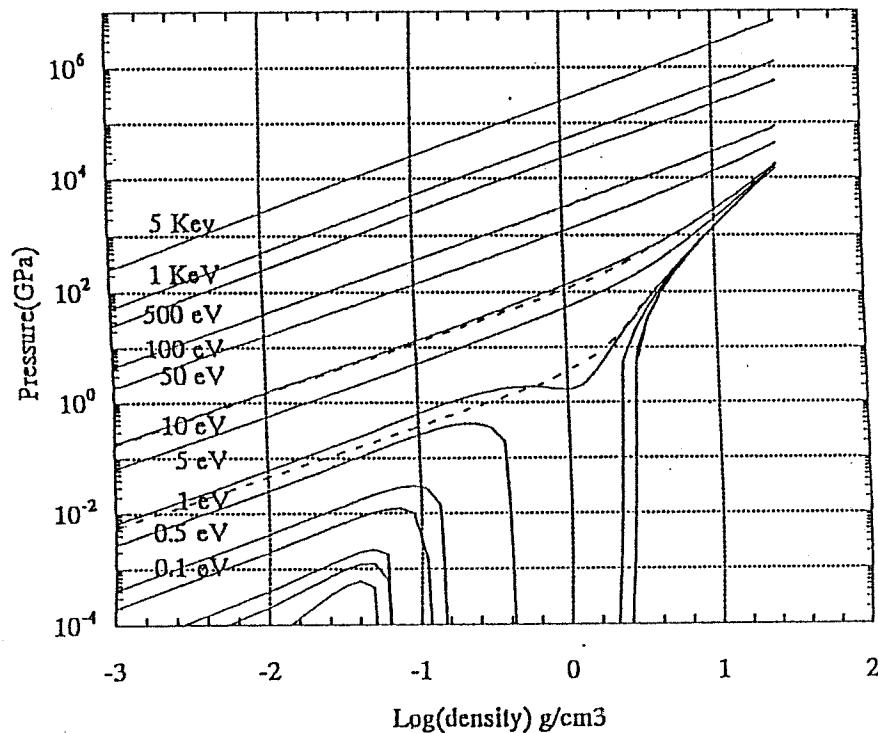
- SESAME / QEoS

$$E = E(\rho, T), P = P(\rho, T)$$

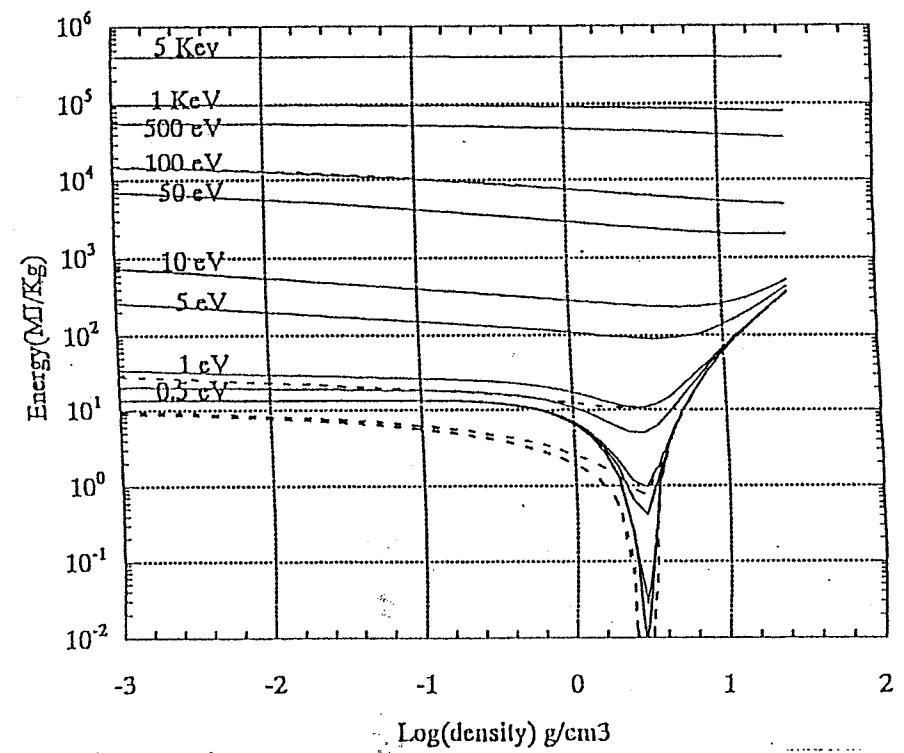
E : Internal energy P : Pressure ρ : Density T : Temperature

Pressure

Internal Energy



Aluminum



line : QEoS

dot line : SESAME(ID = 3718)

Transportation coefficients

Based on the dense plasma theor.

- electrical conductivity(σ)
- thermal conductivity(K)
- absorption coefficient(A)
- skin layer depth(l)

- K & σ_0

TKN model

(σ_0 : electrical conductivity in dc limit)

- σ

Drude model

$$\sigma(\omega) = \omega_p^2 / 4\pi(v_{ei} - \omega)$$

$$v_{ei} = Z^* n_i e^2 / m \sigma_0$$

- l & A

$$A_c e^{-(l+iv)z} = \int dk \frac{e^{ikz}}{\omega^2/c^2 - k^2 + i(4\pi\omega/c^2)\sigma(\omega)}$$

$$A = \frac{4 \operatorname{Re}(Z)}{|1 + Z^2|^2}$$

Z : Surface impedance

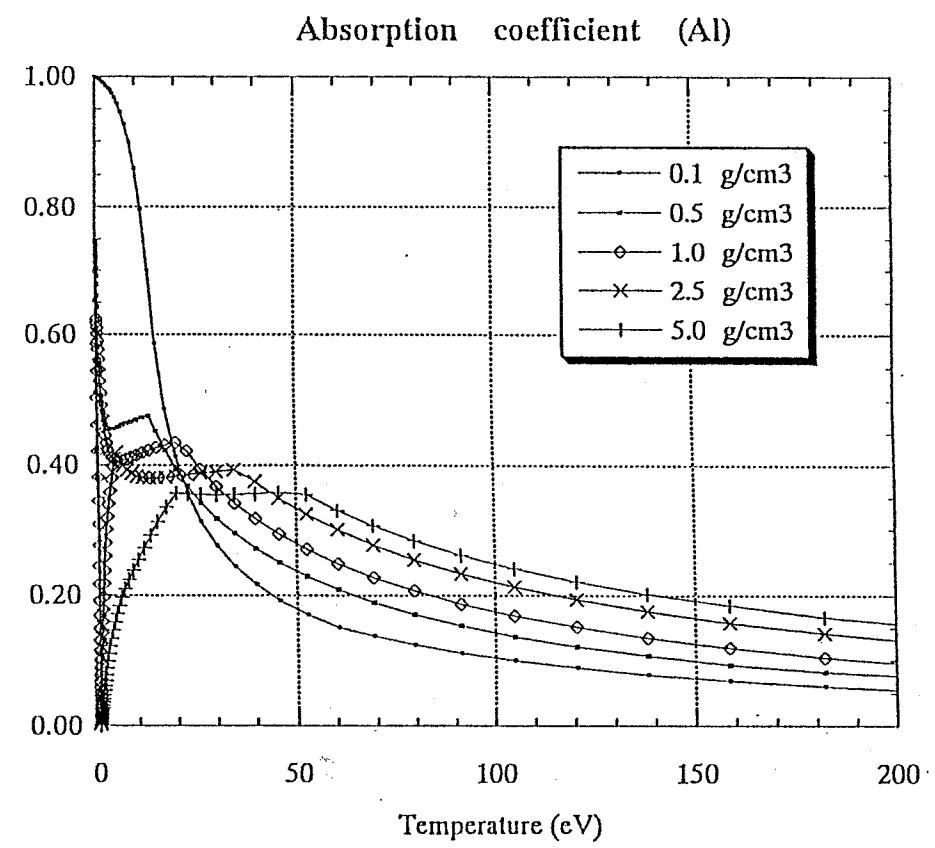
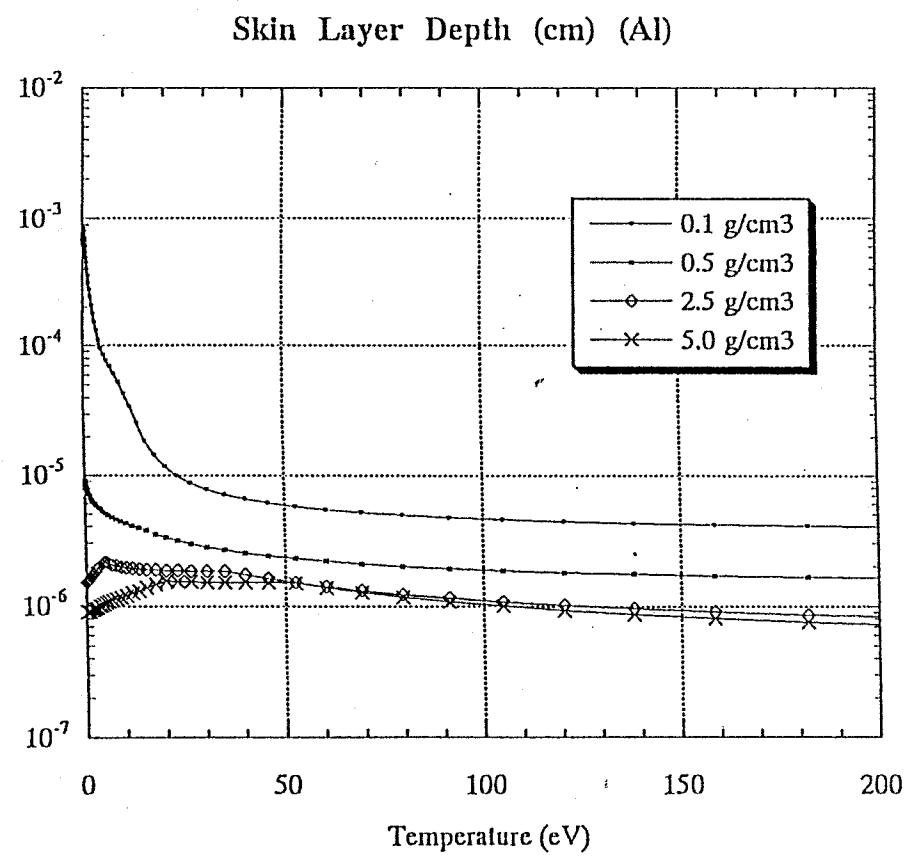
$$(A = \frac{\text{Absorbed Power}}{\text{Total Power}})$$

ω : laser freq.

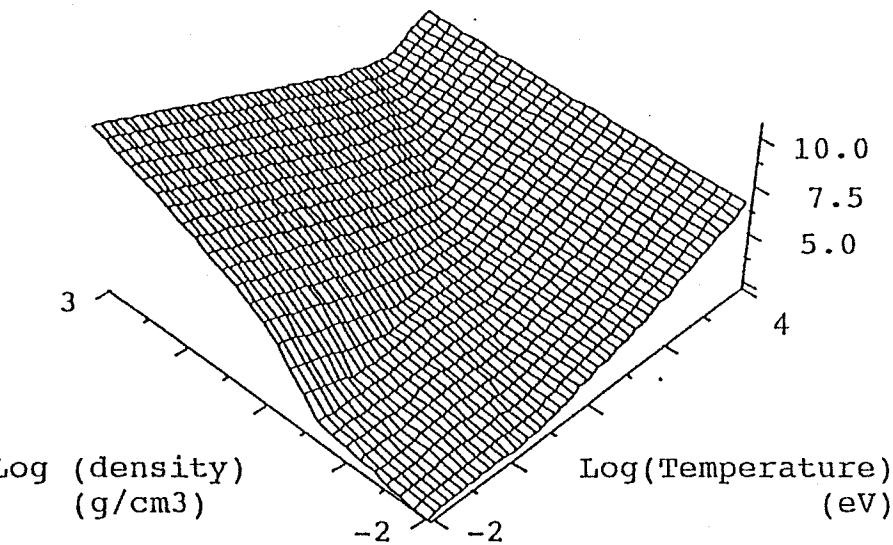
λ : laser wavelength

Z^* : ionization state

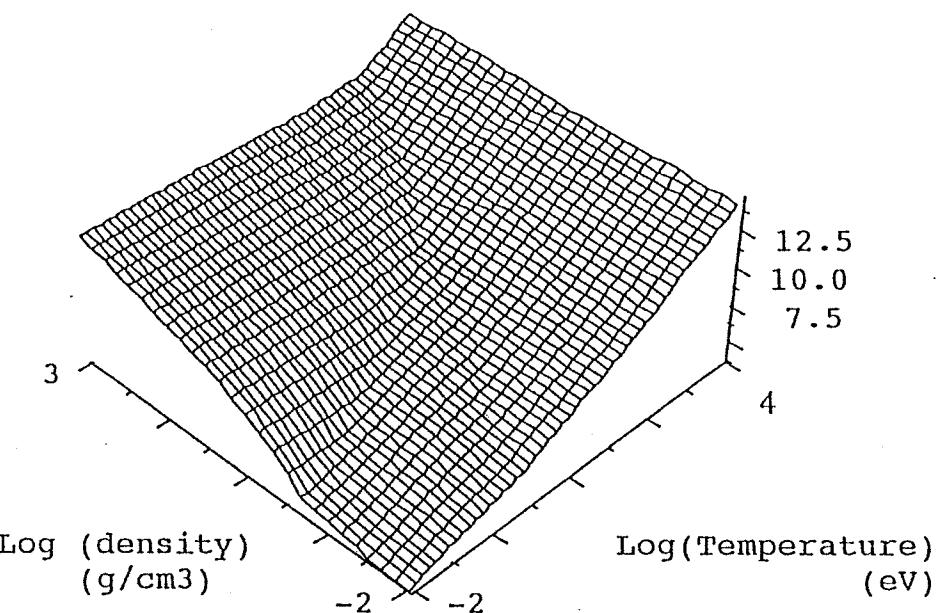
ω_p : plasma freq.



Log (electrical conductivity)
($1/(\text{ohm cm})$)



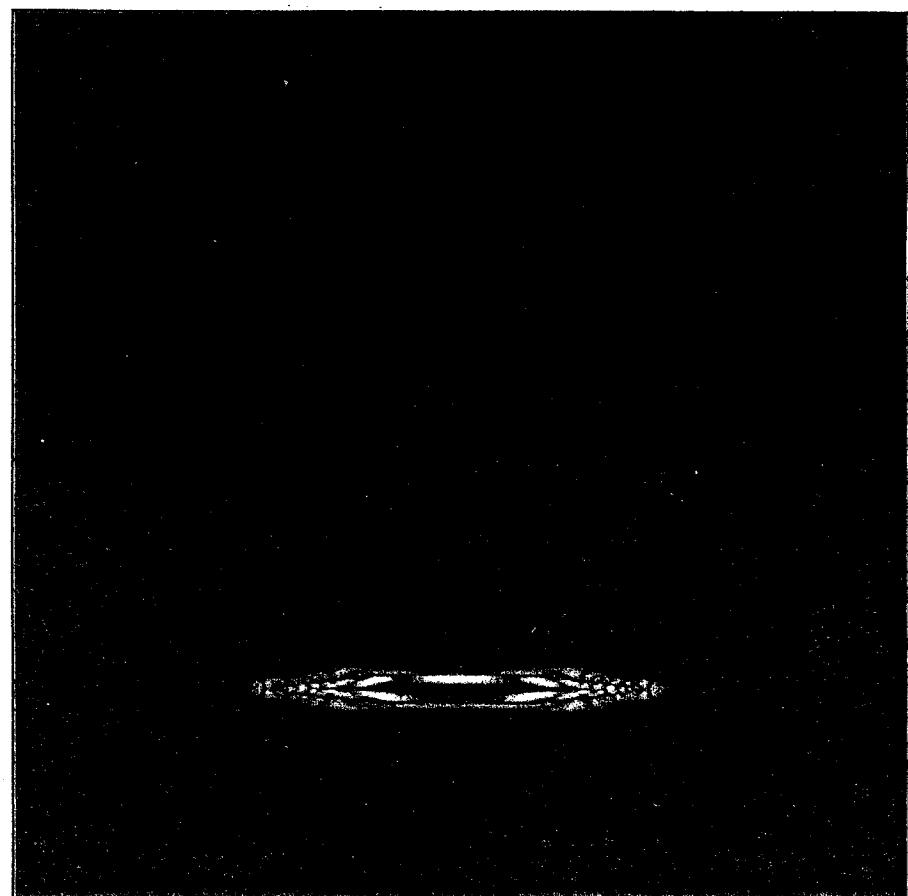
Log (thermal conductivity)
(W/cm keV)



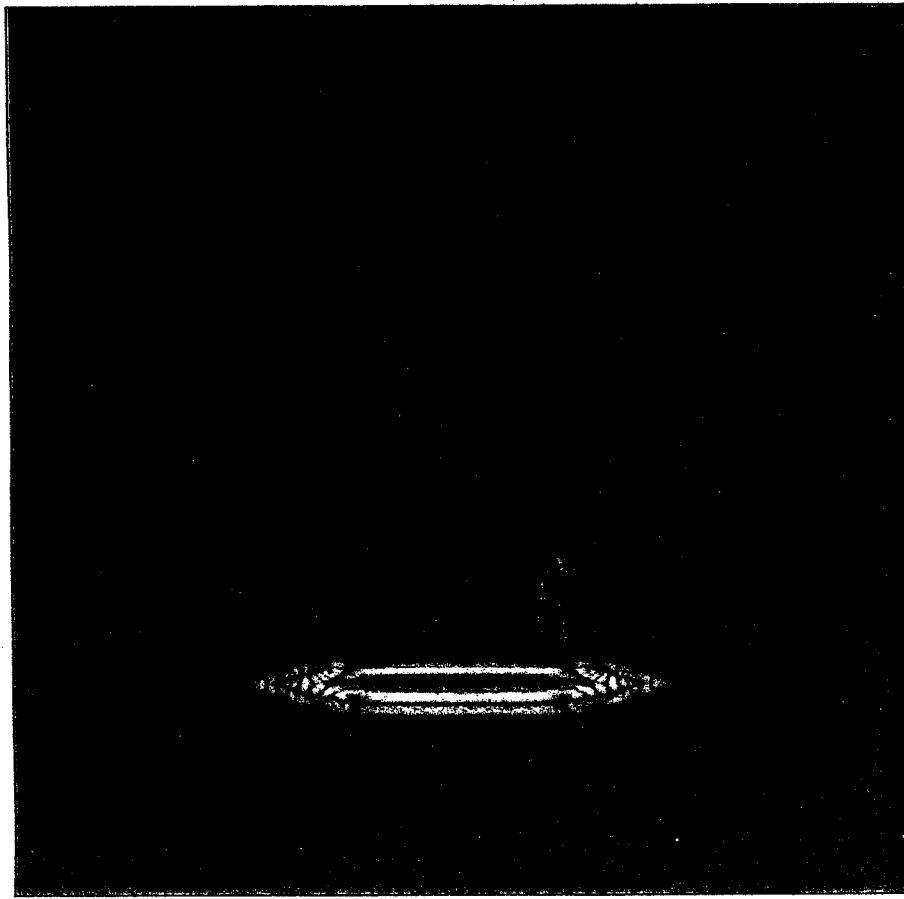
Pressure

unit: $\log_{10}(\text{Pa})$

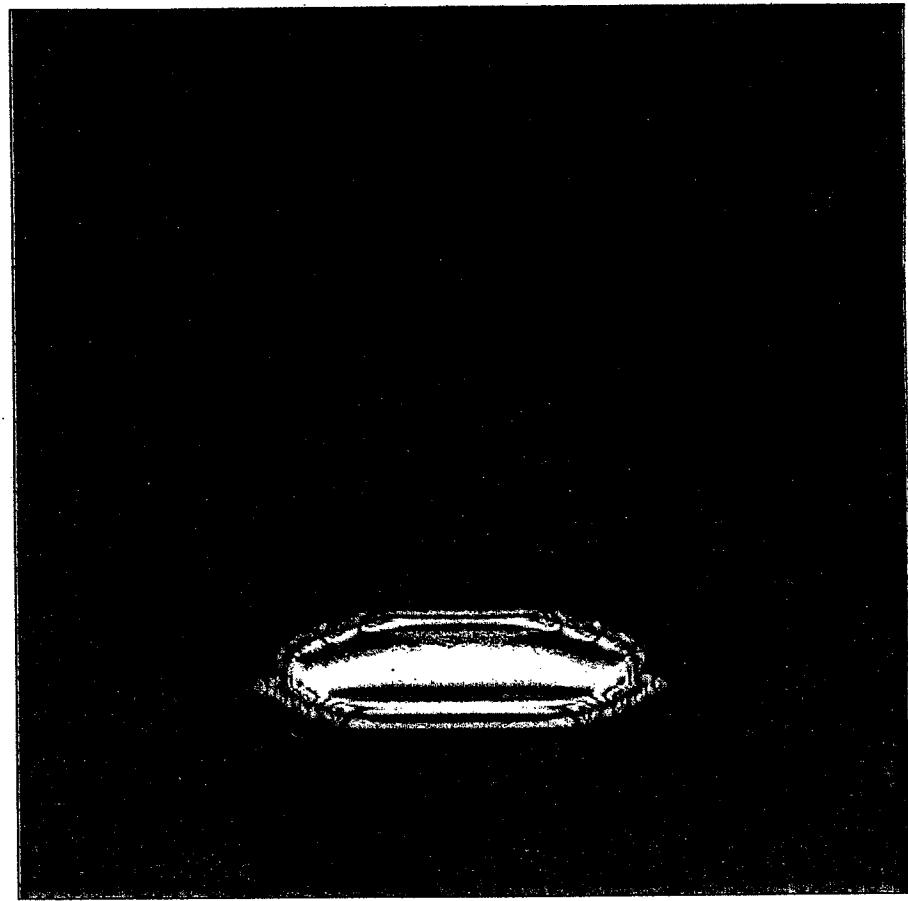
10^3 10^{14} Pa



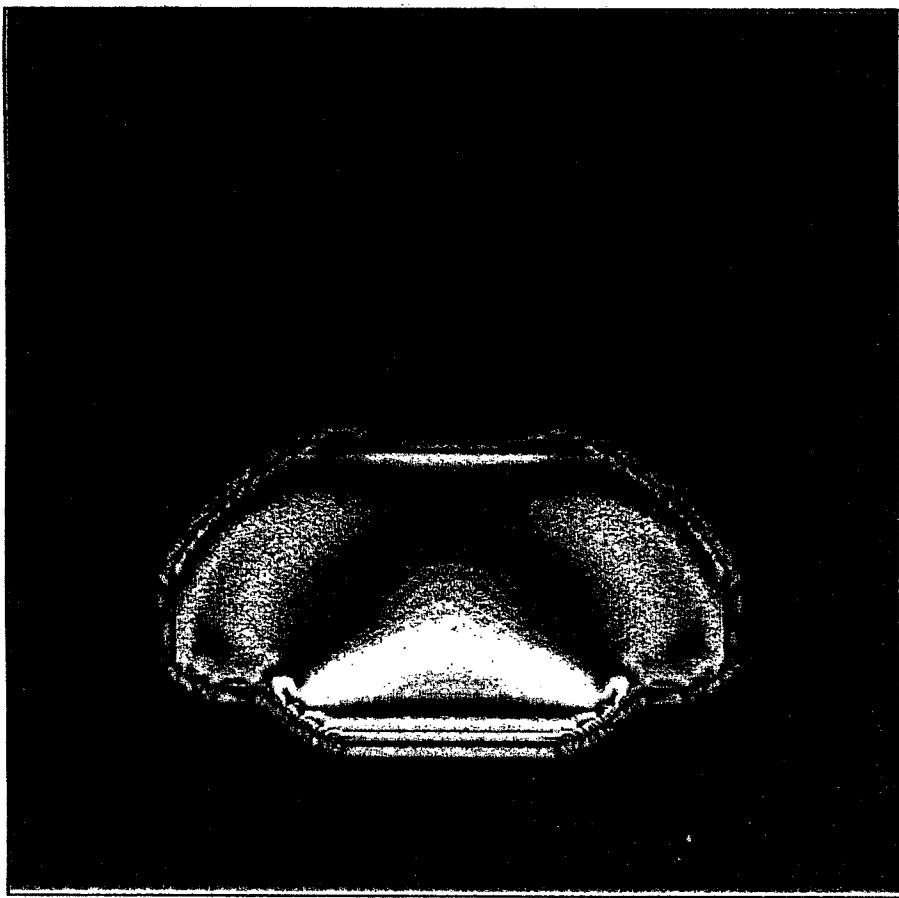
Time = 40fs



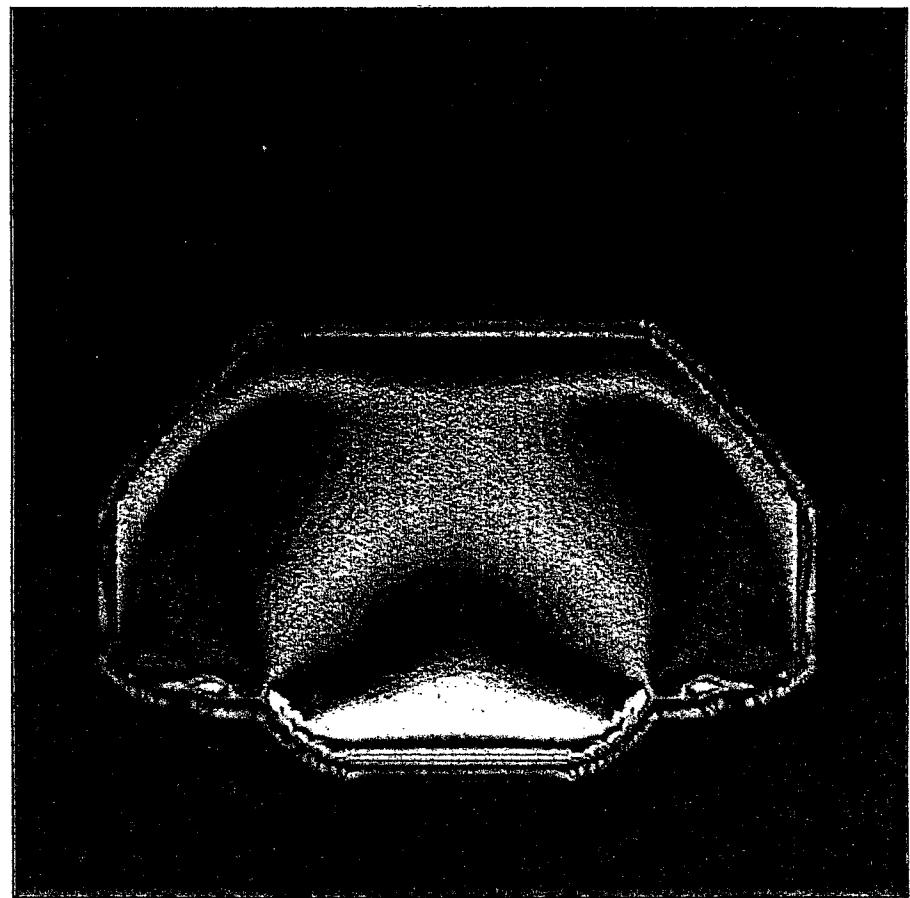
Time = 1 ps



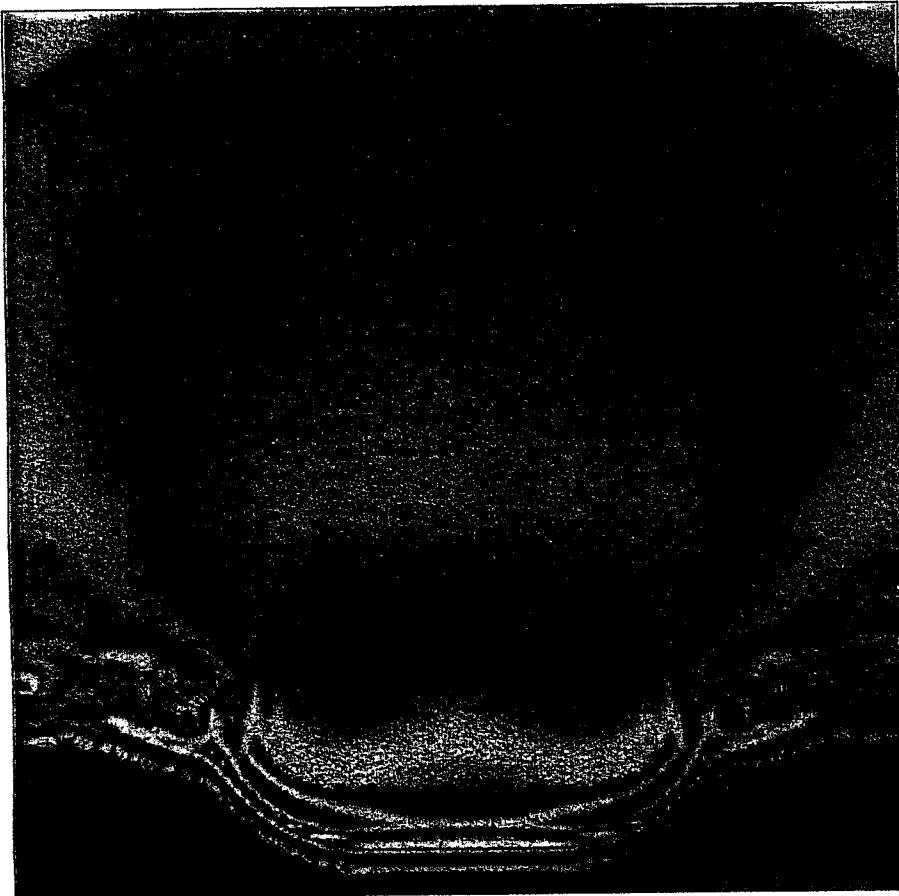
Time = 10 ps



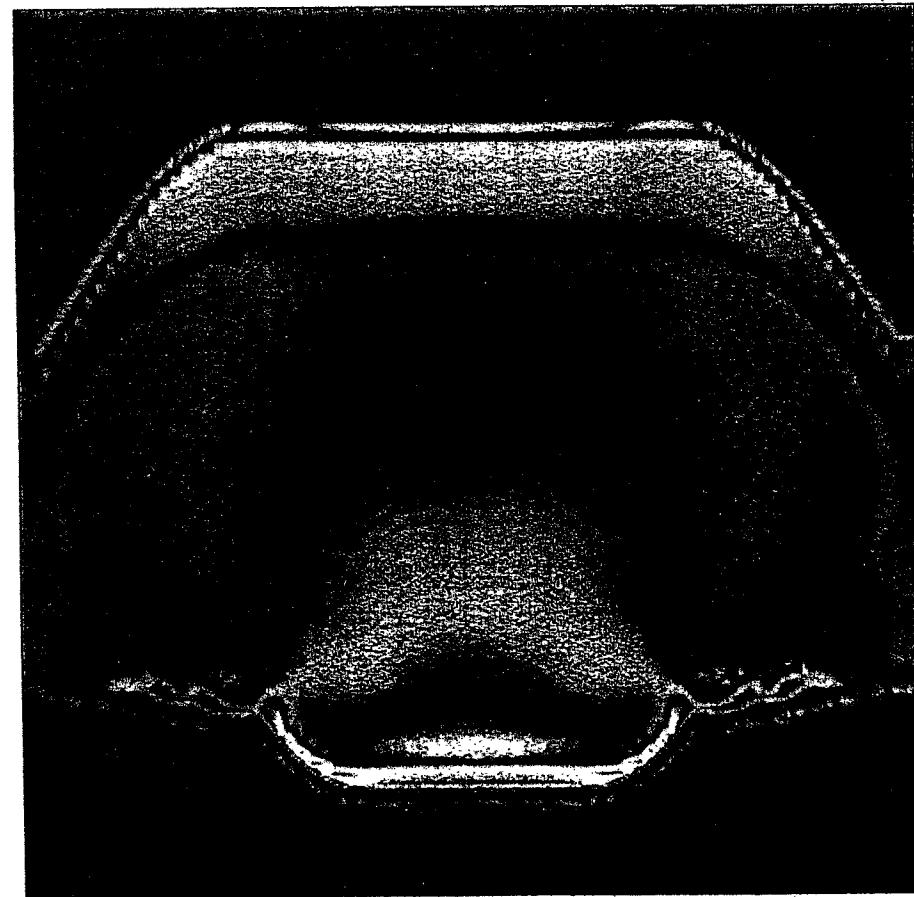
Time = 60 ps



Time = 100 ps



Time = 500 ps



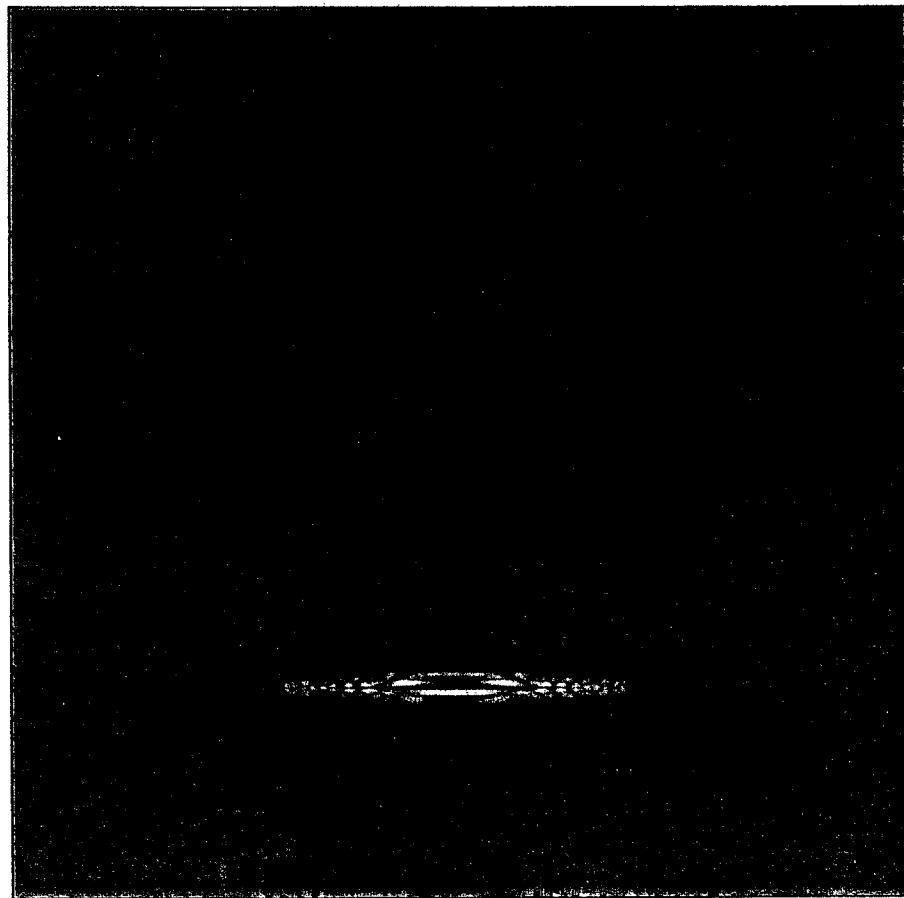
Time = 200 ps

Temperature

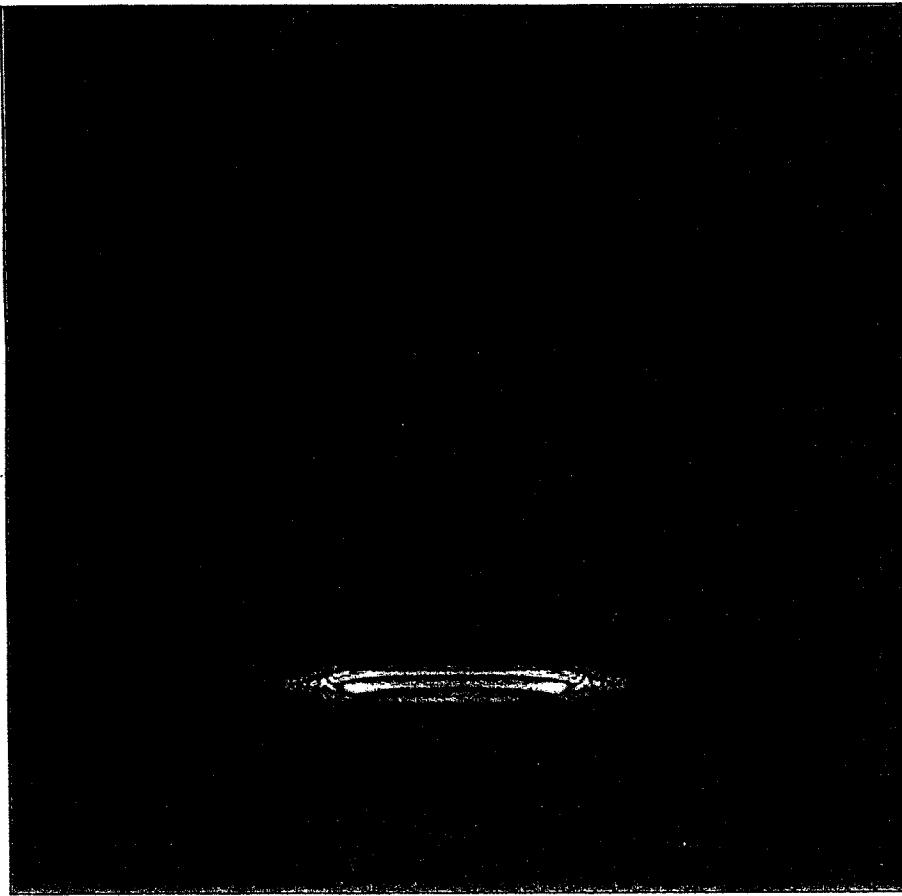
unit: $\log_{10}(K)$



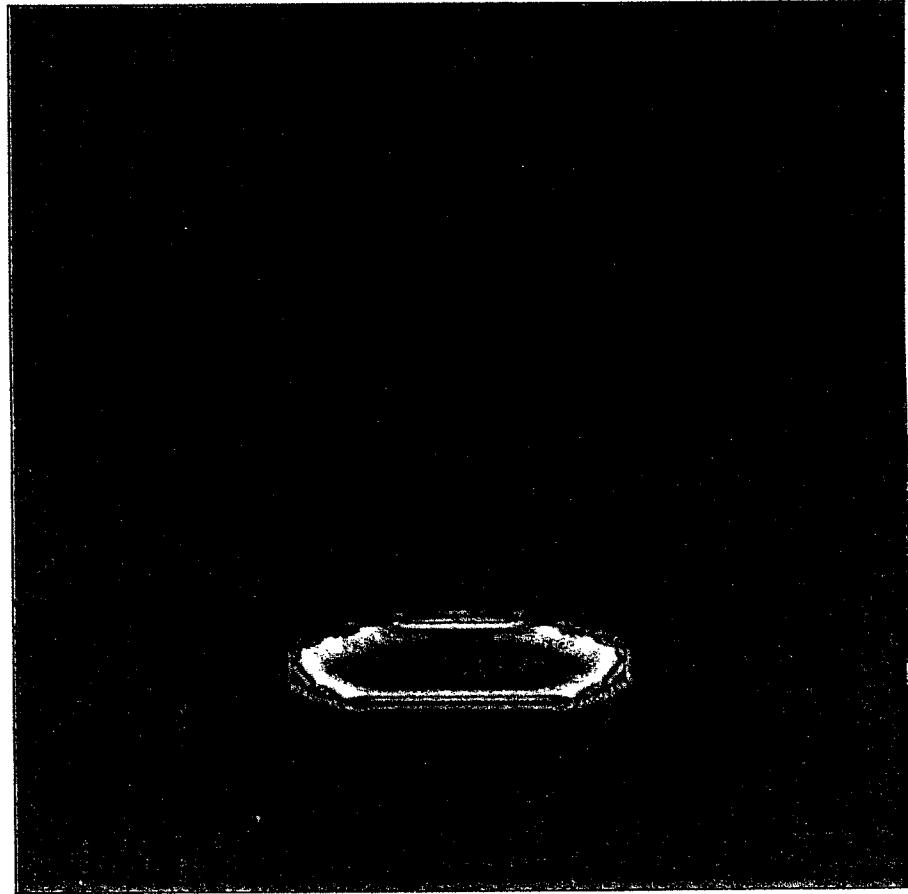
600 10^7 K



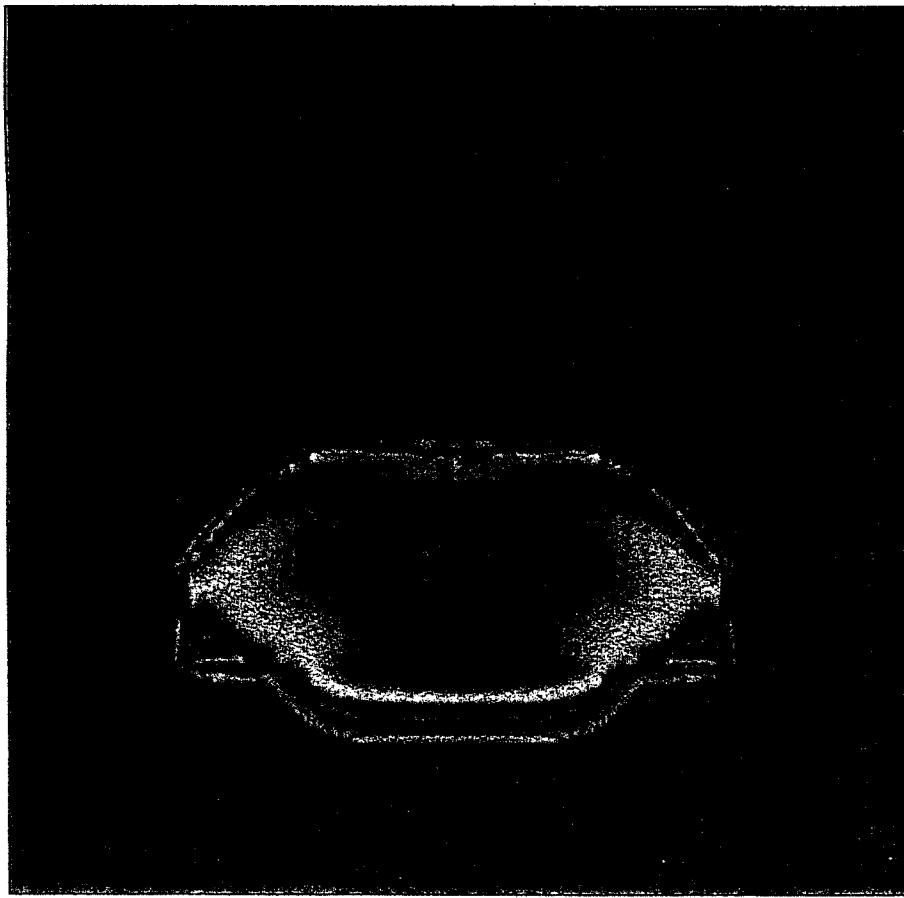
Time = 40fs



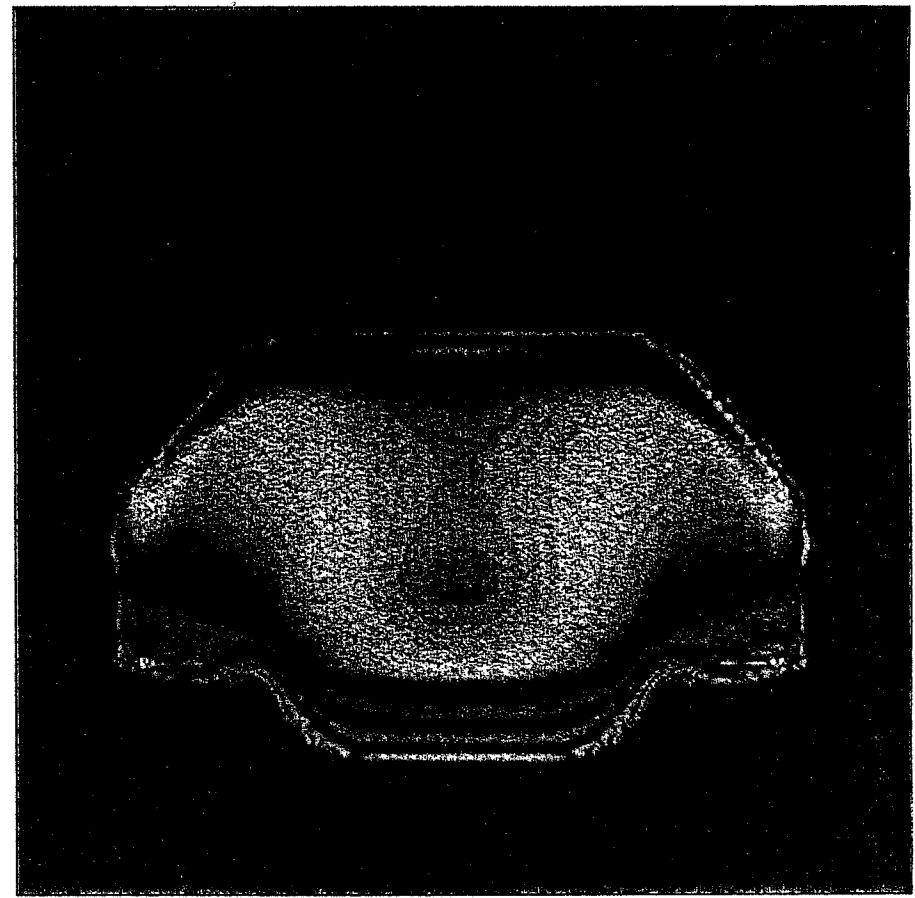
Time = 1 ps



Time = 10 ps



Time = 60 ps



Time = 100 ps

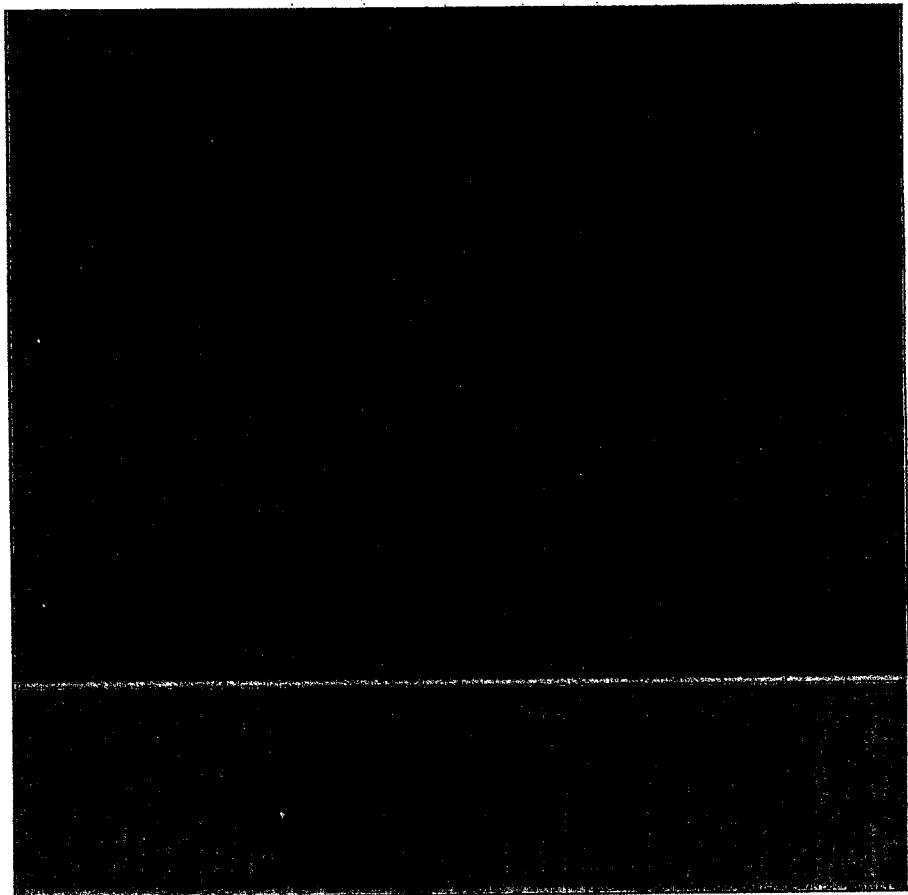
Density

unit: $\log_{10}(\text{kg/m}^3)$

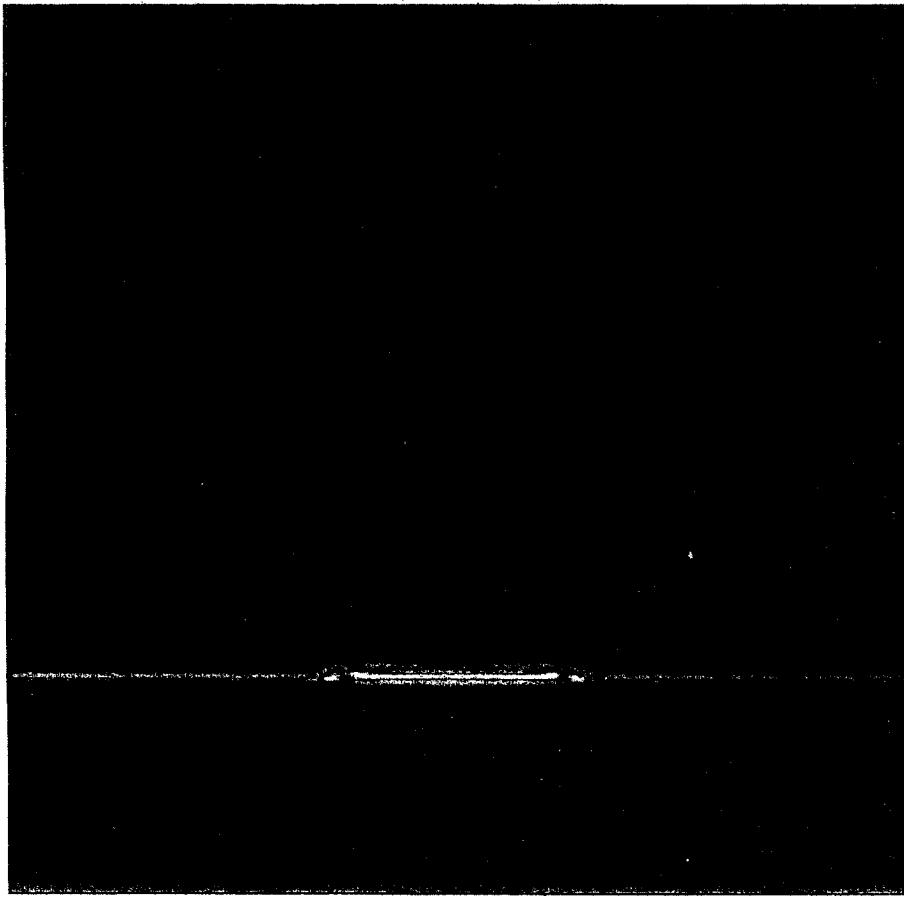


$10^{-0.25}$

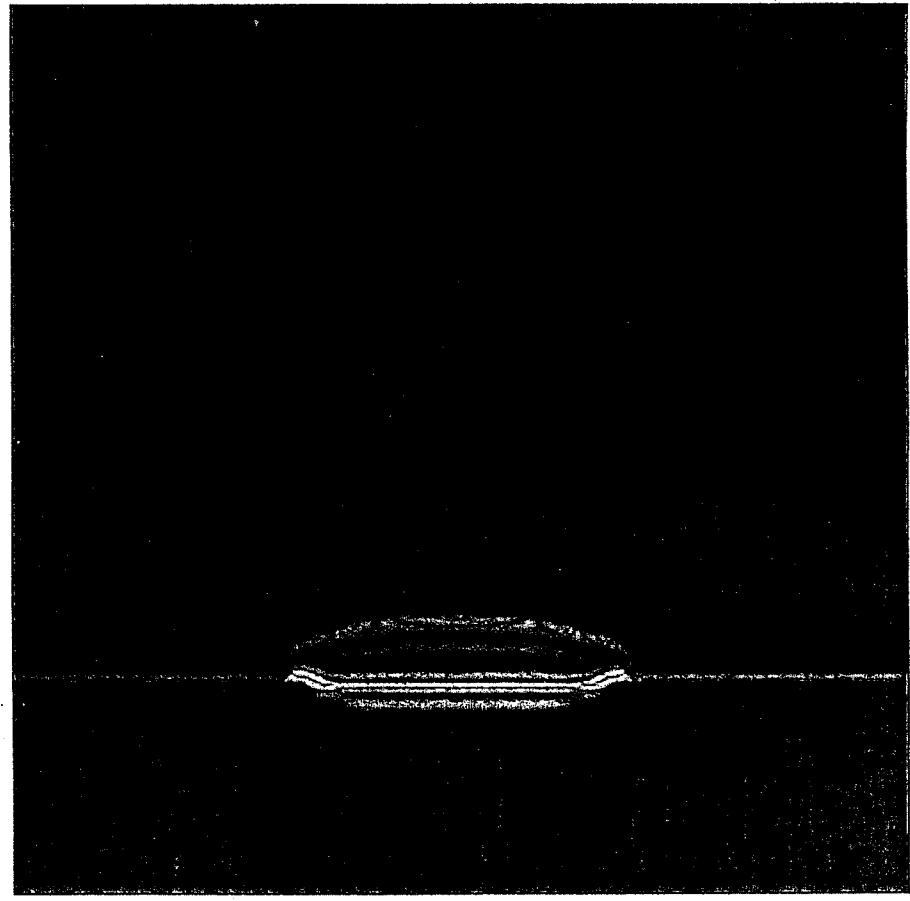
10^4 kg/m^3



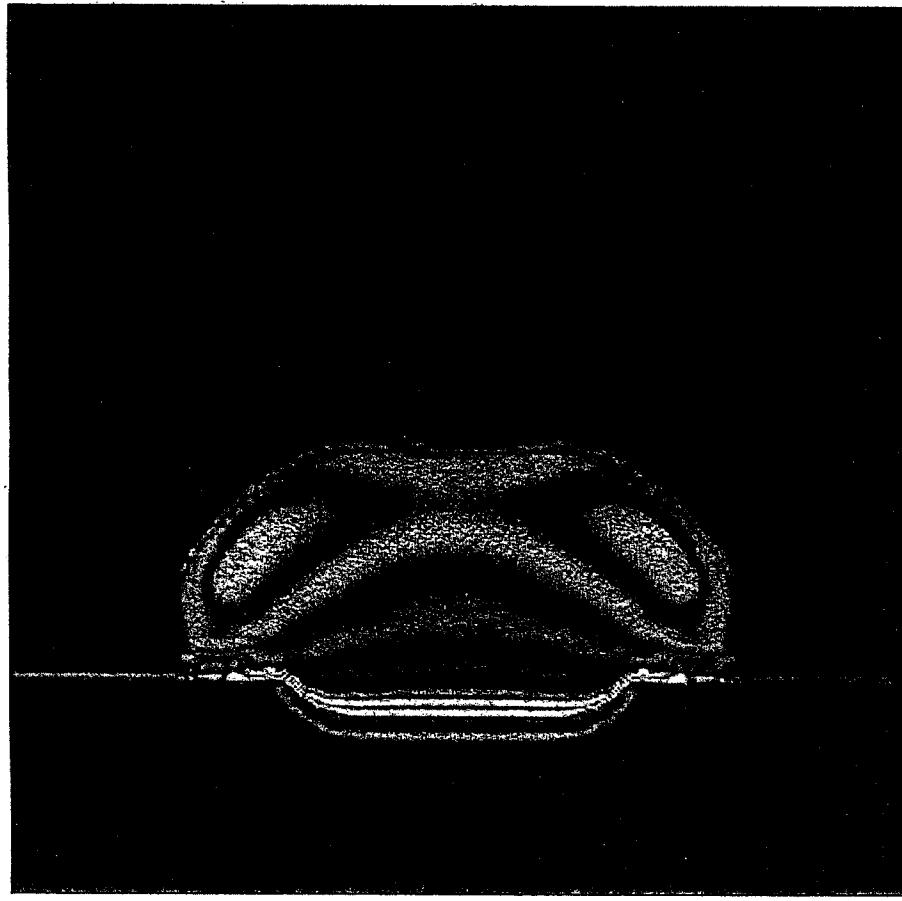
Time = 40fs



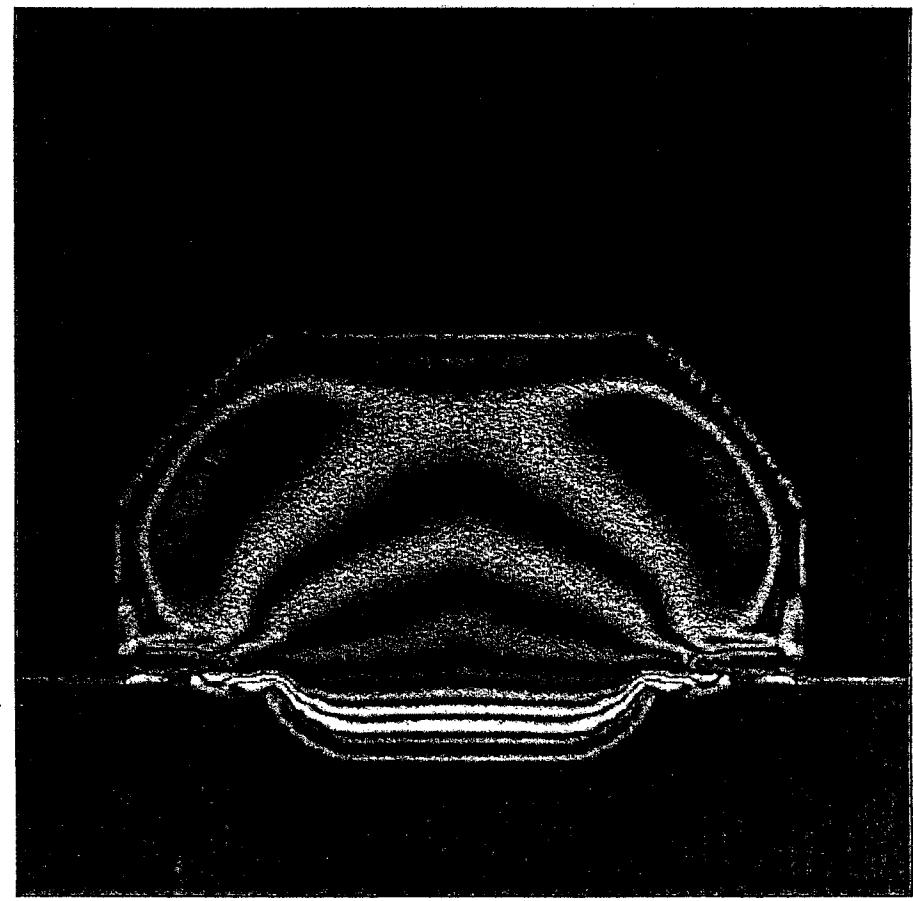
Time = 1 ps



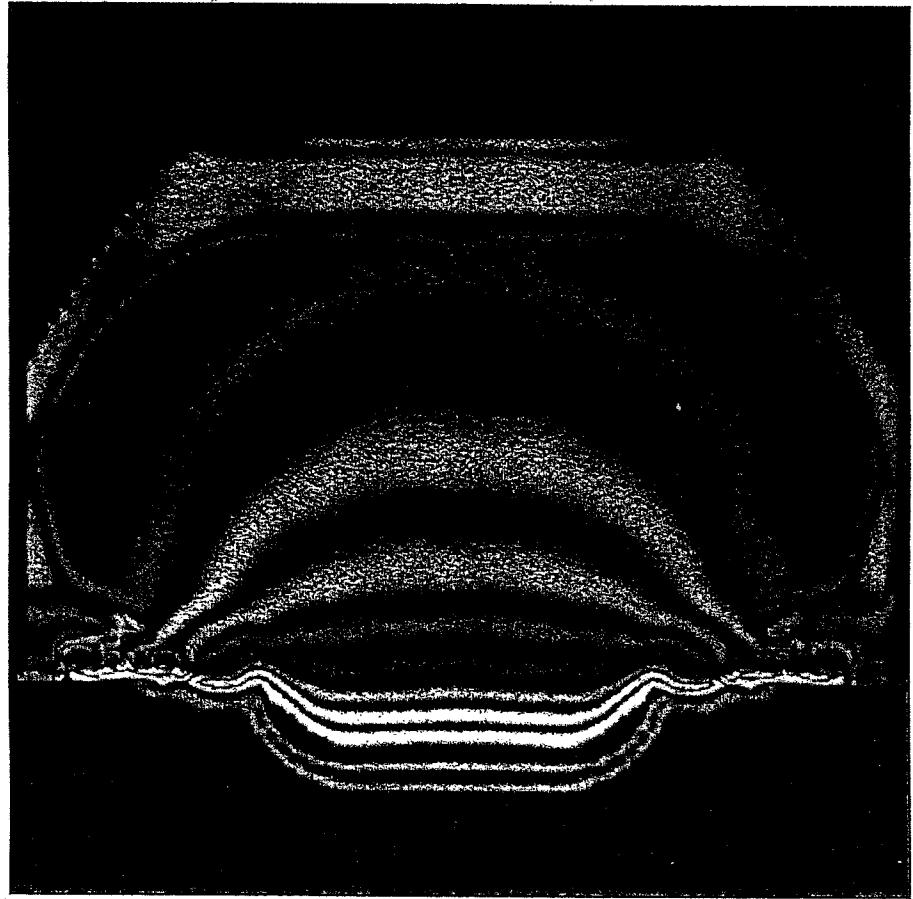
Time = 10 ps



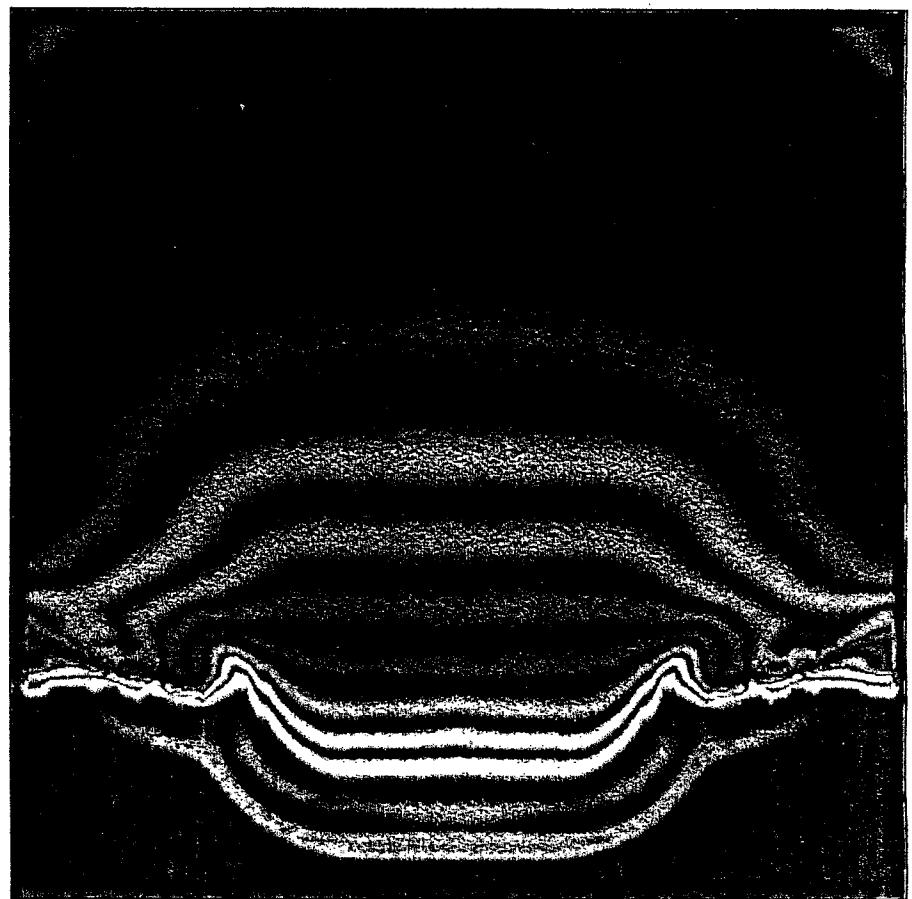
Time = 60 ps



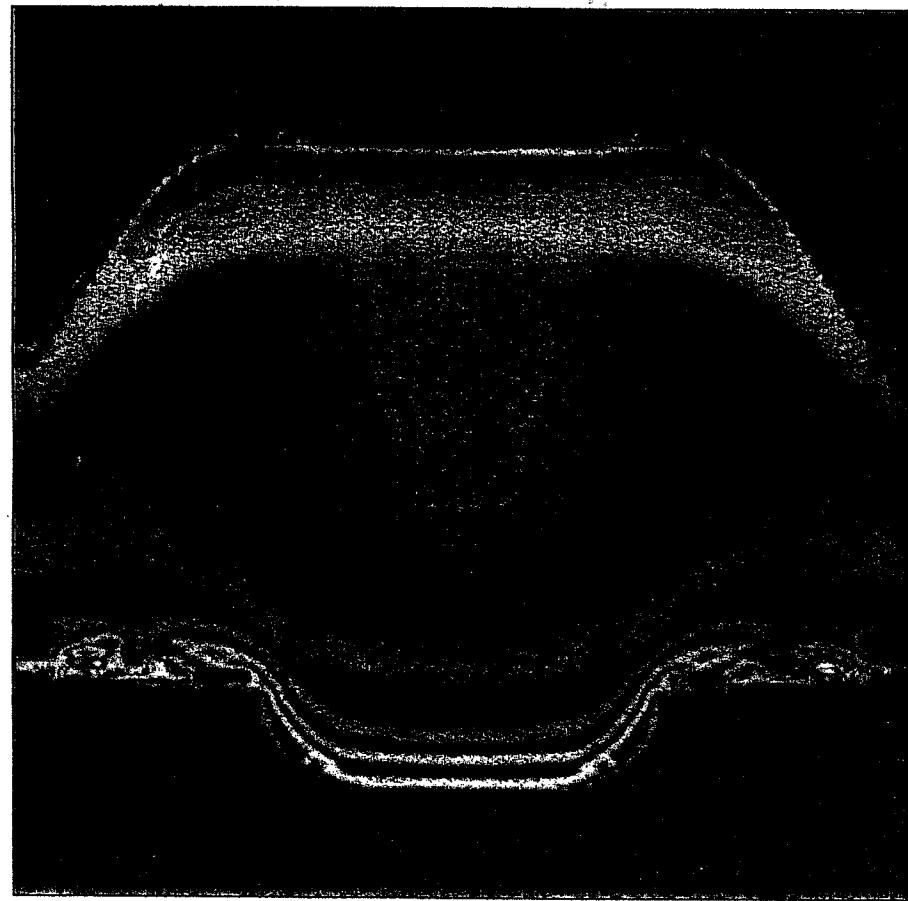
Time = 100 ps



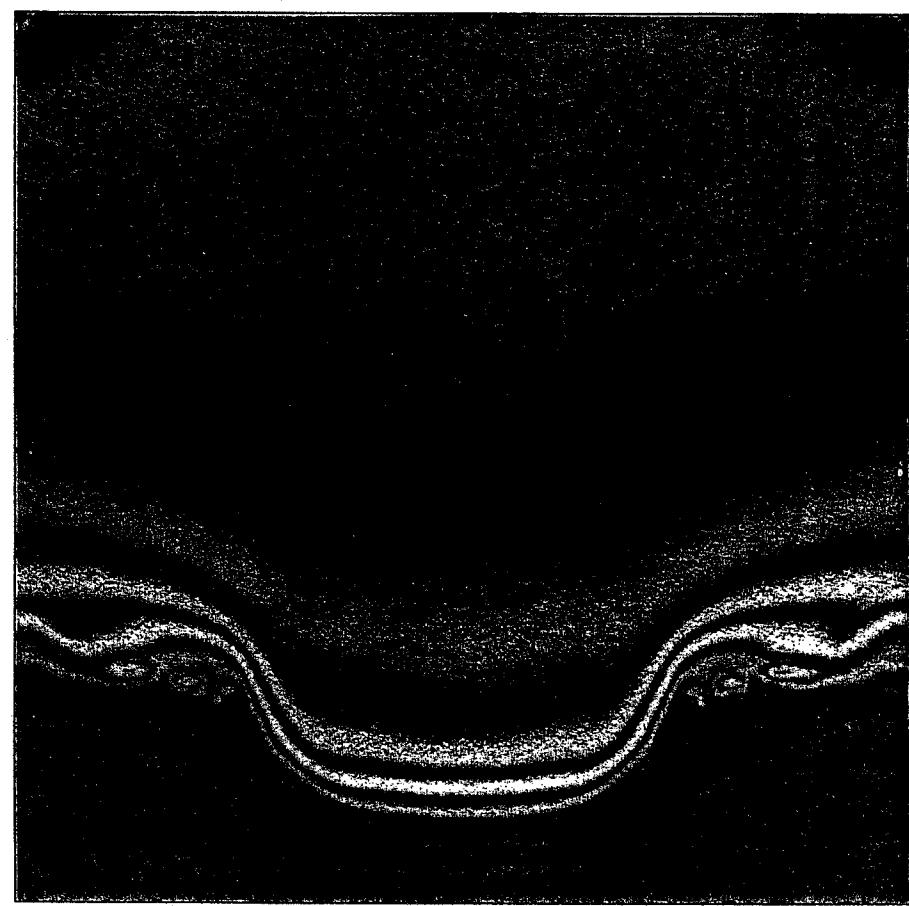
Time = 200 ps



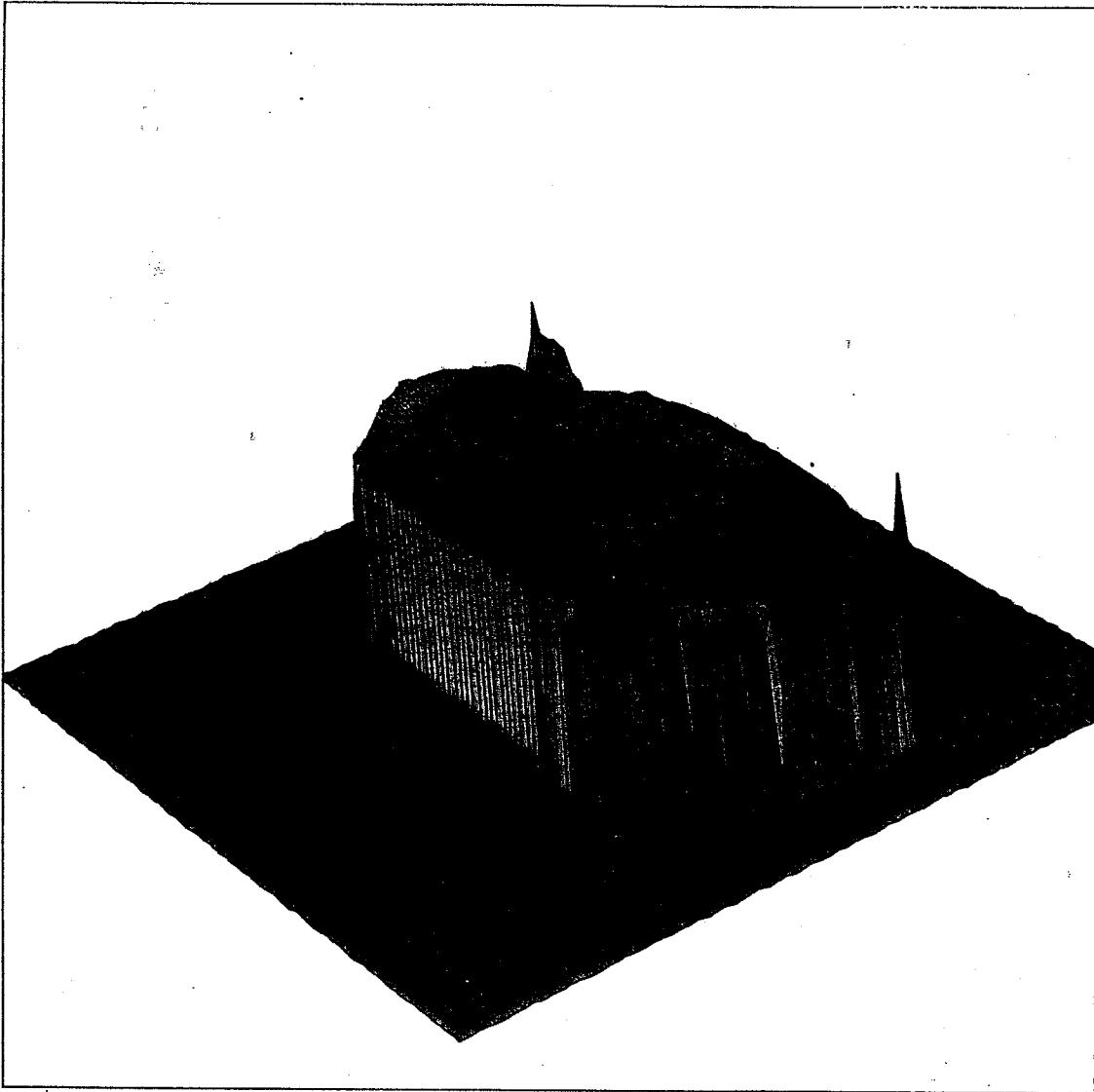
Time = 500 ps



Time = 200 ps



Time = 500 ps

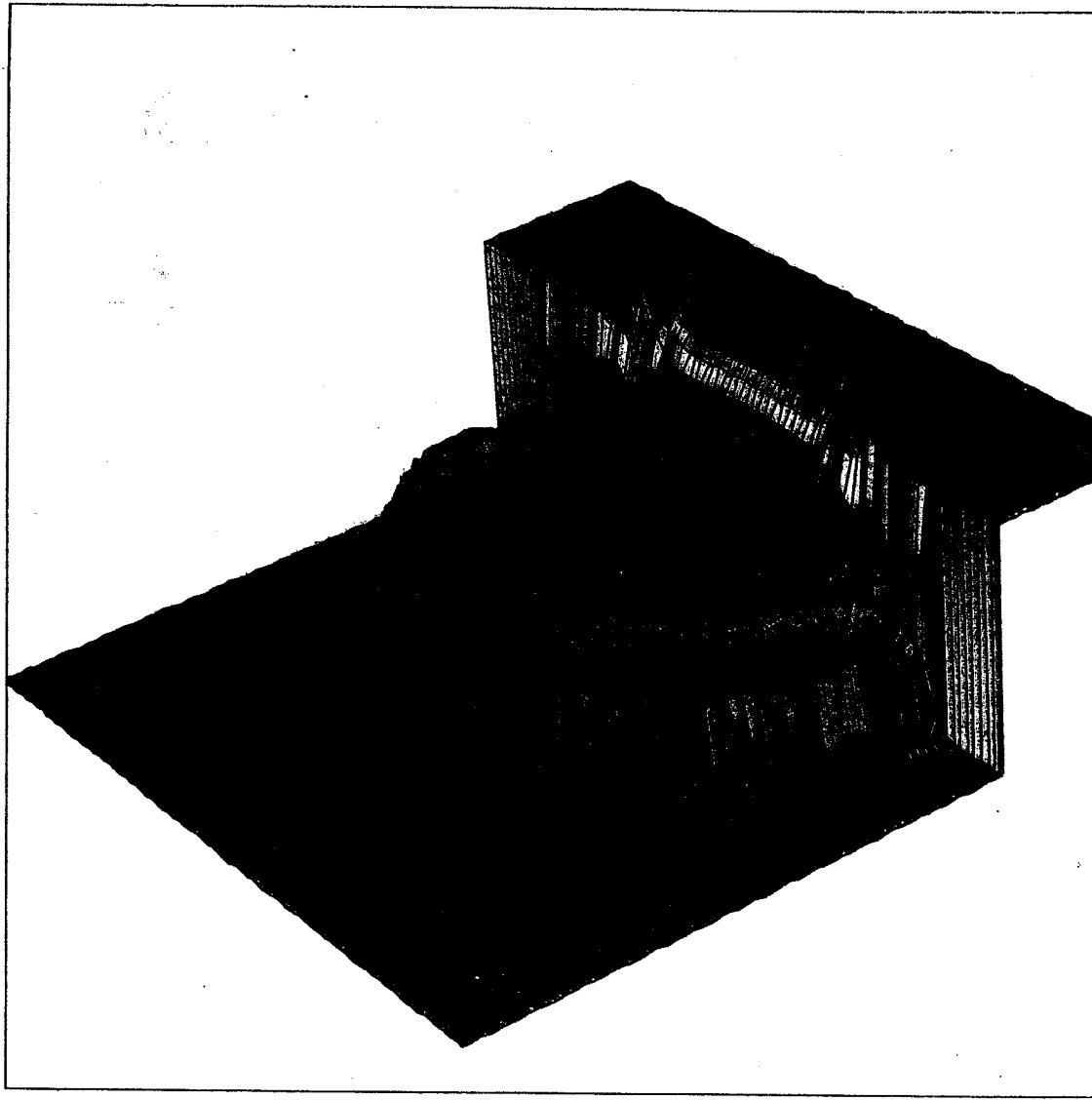


Temperature at time = 100 ps

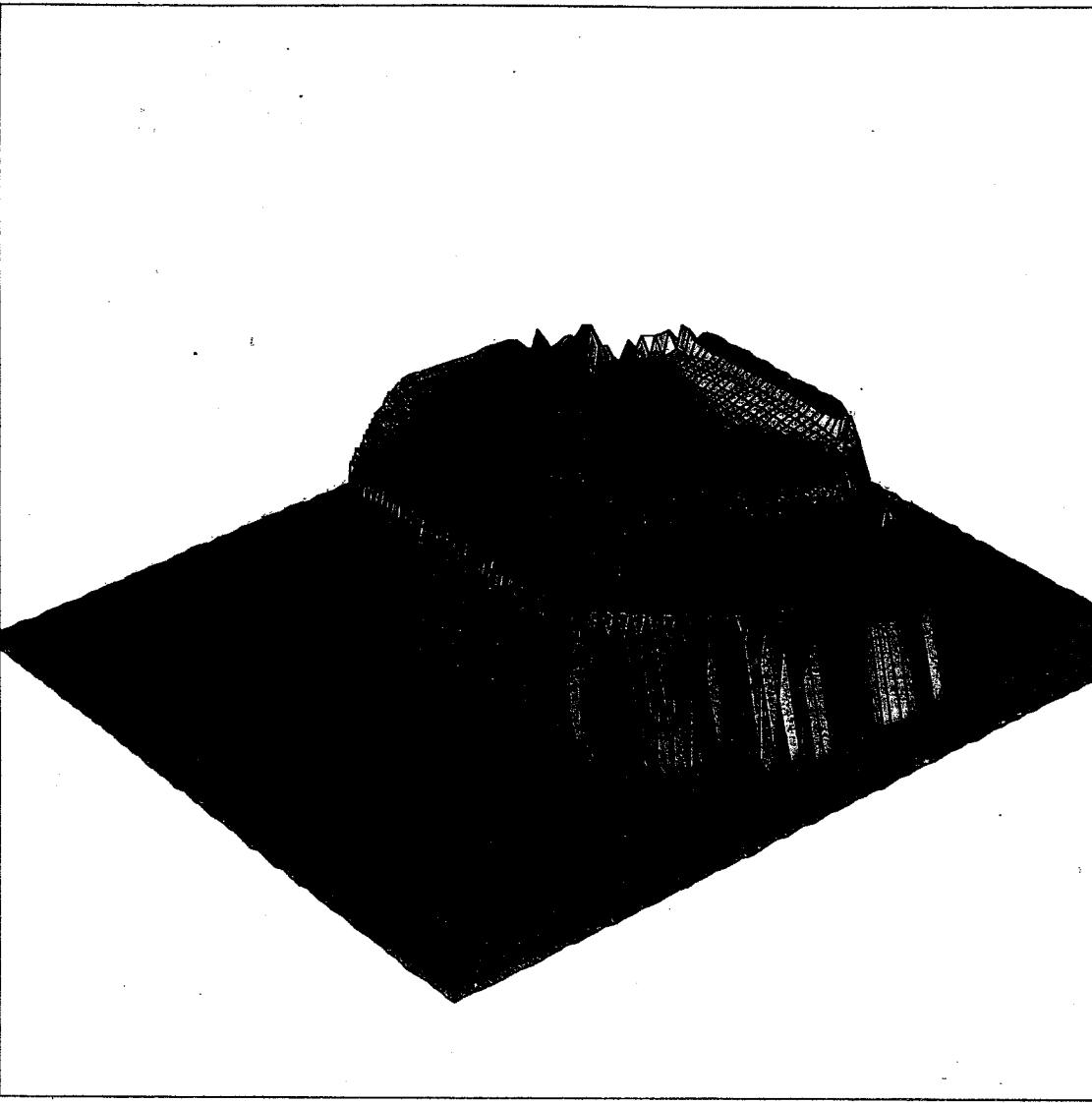
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Density at time = 100 ps



Pressure at time = 100 ps

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Remaining Issues

- (1) Appropriate model for laser-plasma interaction
absorption, refraction in a dense plasma**
- (2) Exact treatment in the solid region
elastic-plastic / viscoelastic model**
- (3) Validation study of the hydrodynamic code
comparison with measurement data**