Numerical Simulation on Thermal Response of Materials Irradiated by High Heat Flux

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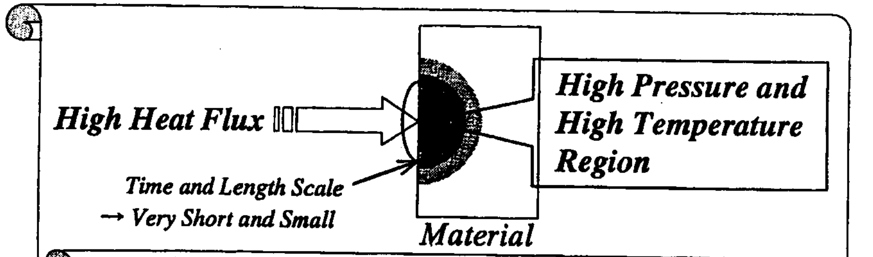
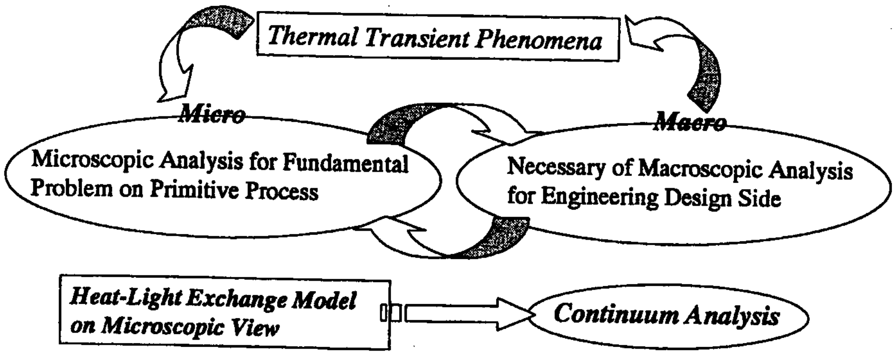
1. *OBJECT*

- # Erosion Damage of Plasma Facing Component in a Fusion Reactor
- # Quality of Laser Assisted Processing of Materials
- # Life Time of Optical Devices Used in Advanced Laser System



Phenomenon of Material Irradiated by High Heat Flux

To estimate these ... ⇨ Micro- and Macroscopic Comprehension of Such Transient Phenomena with a Strong Thermal Non-Equilibrium



Establishment of Macroscopic Universal Solution Considering Microscopic Phenomena

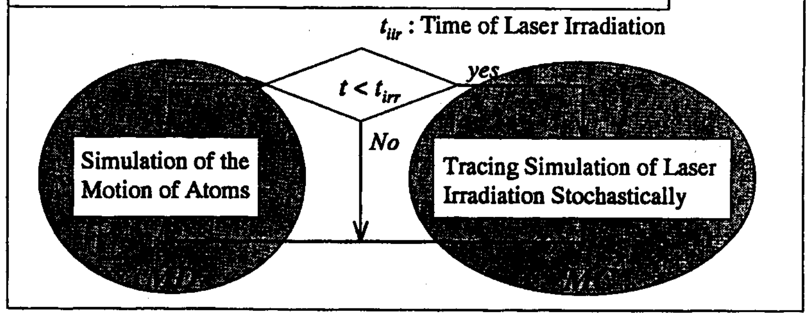
*** Trial Case*

- *Micro Simulation* ⟶ *Molecular Dynamics / Monte Carlo Method (MD/MC)*
- *Macro Simulation* ⟶ *Cubic Interpolated Pseudo-particle Method (CIP)*
- *Target Material* ⟶ *Thin Aluminum Foil* (~ nm)
- *High Heat Flux* ⟶ *High Power Ultra-Short Pulsed Laser* (fs ~ ps)

2. *SIMULATION METOD*

2-1. *Micro Simulation using MD/MC*

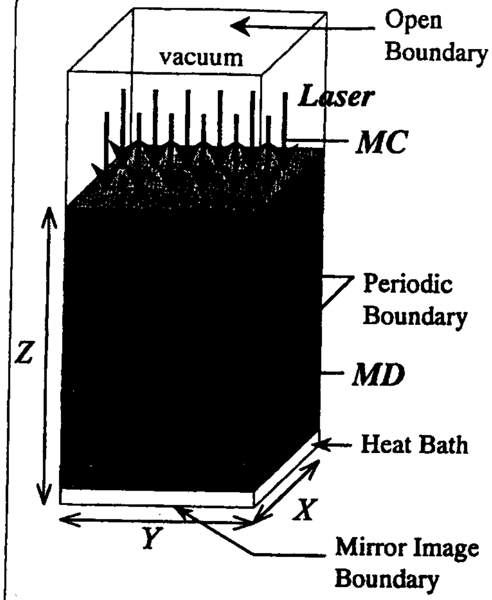
● *Simplified Flow Chart of MD/MC Simulation*



● *Equation of the Motion*

$$m\frac{d\mathbf{v}_i}{dt} = \mathbf{F}_i = -\sum_{j \neq i} \frac{\partial E_{tot}}{\partial \mathbf{r}_{ij}}$$

- m_i : Mass of the *i*-th Atom
- $\mathbf{v}_i$: Velocity of the *i*-th Atom
- $\mathbf{F}_i$: Force Acting on the *i*-th Atom
- $\mathbf{r}_{ij}$: Distance between the *i*-th and *j*-th Atom
- E_{tot} : Potential Function



$X = Y = 11.2$ [nm], $Z = 49.2$ [nm]

Total Number of Atoms = 380,000

Material : Al, $T_0 = 300$ [K]

Simulation System and Boundary Conditions for MD/MC Simulation

● *Inter-Atomic Potential*

Many-Body Potential Function as Inter-Atomic Potential

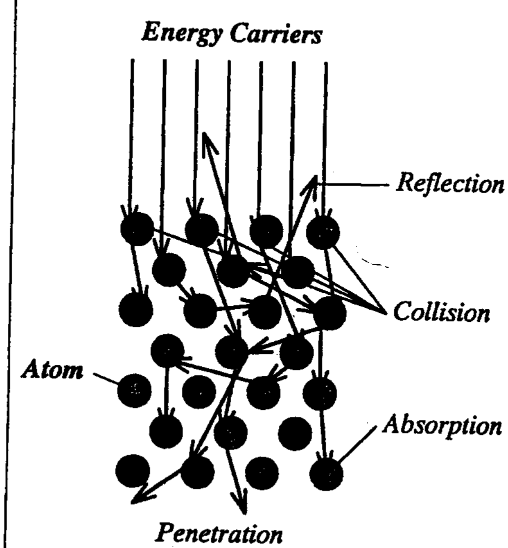
⇨ **<u>Embedded Atom Method</u>** (*EAM*) [Daw&Baskes, 1984]

$$E_{tot} = \sum_i F_i^{emb}(\rho_i) + \frac{1}{2}\sum_i \sum_{j \neq i} \phi_{ij}(r_{ij})$$

- E_{tot} : a total energy of the system
- F_i^{emb} : an embedded energy of atom
- ρ_i : an electron density
- ϕ_{ij} : a two-body central potential
- r_{ij} : an inter-atomic distance

** *Advantage of Many-body Potential over Pair Potential*

⇨ This potential overcomes a disadvantage of pair-potential such that it cannot reproduce properties of surface of transition metal



A Conceptual Diagram of Laser Model for MD/MC Simulation

● *Laser Model*

⇨ ***" Energy Carrier "***

Assumption : 1. This is a particle with no mass but a given energy.

2. These energy carriers transfer only energy.

→ Various Optical Properties ✕

Energy Carriers Move and Collide with Atoms ...

Collision → *test particle MC* → <u>Absorption</u> / <u>Scattering</u>

Case	I_0[W/m^2]	t_s[ps]	Δt[s]	E_0[J/m^2]
1	1.0×10^{14}	0.1	0.5×10^{-15}	10
2	1.0×10^{15}	0.1	0.5×10^{-15}	100
3	1.0×10^{16}	0.1	0.1×10^{-15}	1000

The Condition of Laser Irradiation

I_0 is the heat flux, t_s the pulse duration, Δt the time step, and E_0 the total incident energy.

2-2. *Macro Simulation using CIP*

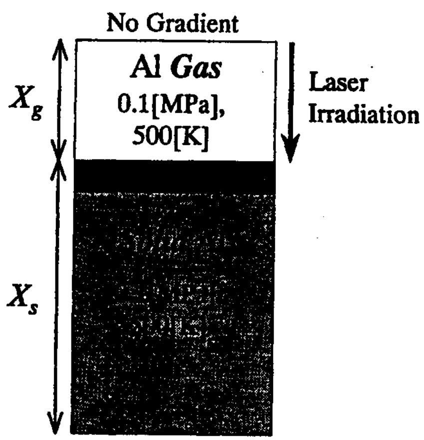
※ *We treat this analysis as 1-dimensional problem.*

● *Governing Equations*

- Equation of Continuity : $\dfrac{D\rho}{Dt} = -\rho \dfrac{\partial u_i}{\partial x_i}$
- Equation of Motion : $\dfrac{Du_i}{Dt} = -\dfrac{1}{\rho}\dfrac{\partial P}{\partial x_i} + \dfrac{1}{\rho}\dfrac{\partial S_{ij}}{\partial x_j}$
- Equation of Energy : $\dfrac{De}{Dt} = \dfrac{1}{\rho} S_{ij} \dfrac{\partial u_i}{\partial x_j} - \dfrac{1}{\rho} P \dfrac{\partial u_i}{\partial x_i} + \dfrac{\partial}{\partial x_i}\left(\dfrac{\kappa}{\rho}\dfrac{\partial T}{\partial x_i}\right) + \dfrac{Q}{\rho}$

⇨ ***We use equation of energy with pressure as dependent variable.***

$$\frac{DP}{Dt} = \frac{1}{\rho\left(\frac{\partial e}{\partial P}\right)_\rho}\left[-P + \rho^2\left(\frac{\partial e}{\partial \rho}\right)_P\right]\frac{\partial u_i}{\partial x_i} + \frac{1}{\rho\left(\frac{\partial e}{\partial P}\right)_\rho}\left[S_{ij}\frac{\partial u_i}{\partial x_j} + \frac{\partial}{\partial x_i}\left(\kappa\frac{\partial T}{\partial x_i}\right) + Q\right]$$



$u = 0$[m/s], $P_0 = 0.1$[MPa],
ρ = the value corresponding to 0.1[MPa] and 500[K]

$X_g = 0.5$ [μ m], $X_s = 2.0$ [μ m]

Simulation System and Boundary Conditions for CIP Simulation

Thermodynamic Parameters in Equation of Energy

$\left(\dfrac{\partial e}{\partial P}\right)_\rho$ $\left(\dfrac{\partial e}{\partial \rho}\right)_P$ T — *Equation of State (EOS)*

⇨ ***SESAME Library***

● *Laser Model*

- Strong Heat Generation at the Solid Surface
- Profile of Penetrated Laser Energy

⇨ **Beer's Law**

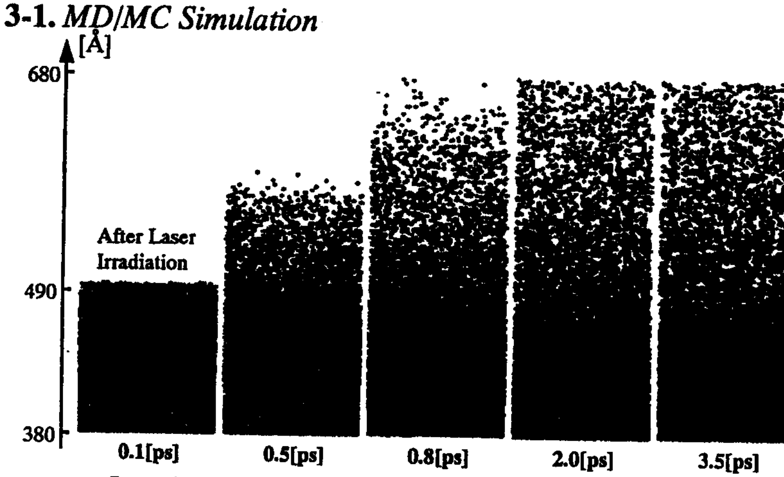
$I = I_0 \exp(-\beta d)$

- I : Intensity of Laser at Depth d
- I_0 : Intensity of Incident Laser
- β : Absorption Coefficient
- d : Absorption Depth

** The condition of laser irradiation is equal to micro simulation.

3. *RESULT*

3-1. *MD/MC Simulation*

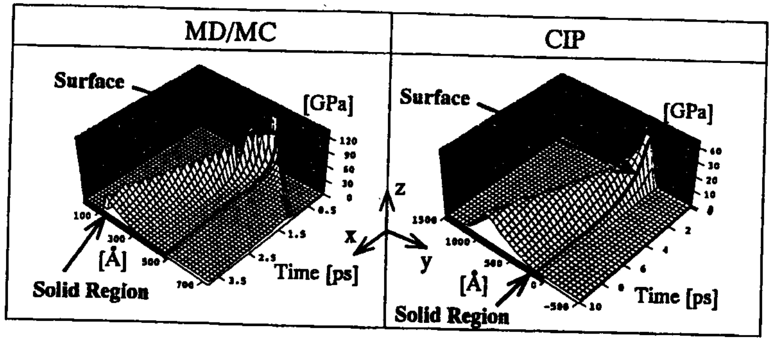


Snapshots of the Atomic Configuration of Al for the Case 3

** Large-scale Phase Change → Just After Laser Irradiation with a Time Lag

- the experimental results of Downer and others ○
- This time lag *may be* the excited time of atoms after absorbing the laser energy.

3-2. *Comparison Between MD/MC and CIP Simulations*



Time History of Depth Direction Profile of **Pressure** *for the* Case 3

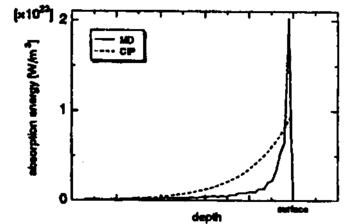
** bold line : initial surface of solid , gray line : initial solid region
x : Time , y : Height , z : Pressure
[・The positive direction of y axis is taken to the height direction]

	MD/MC	*CIP*	
Propagating Velocities of Pressure Wave	about 8,900[m/s]	about 9,000[m/s]	○
Peak of Pressure Wave	about 120[GPa]	about 40[GPa]	×

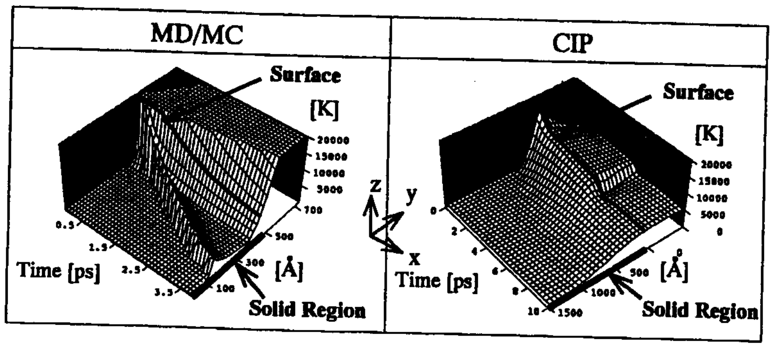
Comparison of Pressure Wave Characteristic

→ Sound Speed in Solid Al = 6,420[m/s] ⇨ *Propagating Velocity is Supersonic*

→ Difference of Peak Value
⇨ *Difference of Laser Model for Both Simulations*



Comparison of the Distribution of
Absorbed Energy for both simulations



Time History of Depth Direction Profile of **Temperature** *for the* Case 3

** bold line : initial surface of solid , gray line : initial solid region
x : Time , y : Height , z : Temperature

 # Thermal Wave** : MD/MC* ○ , ***CIP ×

When thermal disturbance is given to the system during an ultra-short time,
→ *High-Speed Thermal Propagation as a Wave*

** According to Tzou or others ...
Thermal Diffusion Model using ***Fourier Heat Conduction Equation***
→ Heat Transfer as a Wave ×
∴Present Algorithm of ***CIP*** → Non-Equilibrium Thermal Response ×

Additional Term in *Governing Equations* { Thermal Relaxation Process or Volume-Expanding Work }

4. *SUMMARY OF PREVIOUS RESULTS*

Both simulations of MD/MC and CIP are performed on the thermal response of the thin foil irradiated by a high power ultra-short pulsed laser.

Results are summarized as follows :

- The high pressure and temperature regions are formed at the surface of the thin foil irradiated by a high power ultra-short pulsed laser, and the regions propagate towards the inside of it with supersonic velocity.
- From comparison of results of both simulations, the term, which can consider heat transfer based on the volume-expanding work or the thermal relaxation process, is required to reproduce the thermal wave in the macroscopic simulation.

** *Need Item*

***Micro Simulation** (MD/MC)*

1. *Modification Laser Model*
   * Reconsideration for Absorption and Scattering of "*Energy Carrier*"
2. *Electron Effect*
   * Free Electron within Solid of Metal
   * Charged Particle and Electron in Plasma

***Macro Simulation** (CIP)*

1. *Introduction* of *Additional term in Governing Equations*
   ⟹ Prediction of *Thermal Wave*
2. *Improvement of Algorithm*

Experiment

1. *Application of Single Photon Counting Method*
   * Pressure or Thermal Wave at the Rear of Target Material

5. *PROSPECTS FOR NEXT STEP*

** *Our Plan*