SOME NUMERICAL EXPERIMENTS USING MOLECULAR DYNAMICS SIMULATION

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S.H. Park (Hongik University)
J.S. Lee (Seoul National University)

μ Therm

OUTLINES

- Introduction to Molecular Dynamics Simulation
- Visualization of Some Critical Phenomena
  - Vaporization/Formation/Spreading of a Droplet
  - Instability of Liquid Thin Films and LISA process
  - Nanojets
  - Laser Ablation
  - Adhesion and Stiction
- Crystallization of Amorphous Silicon
  - AMFC
  - Voronoi Analysis
  - Heterogeneous Crystallization
- Closing Remarks

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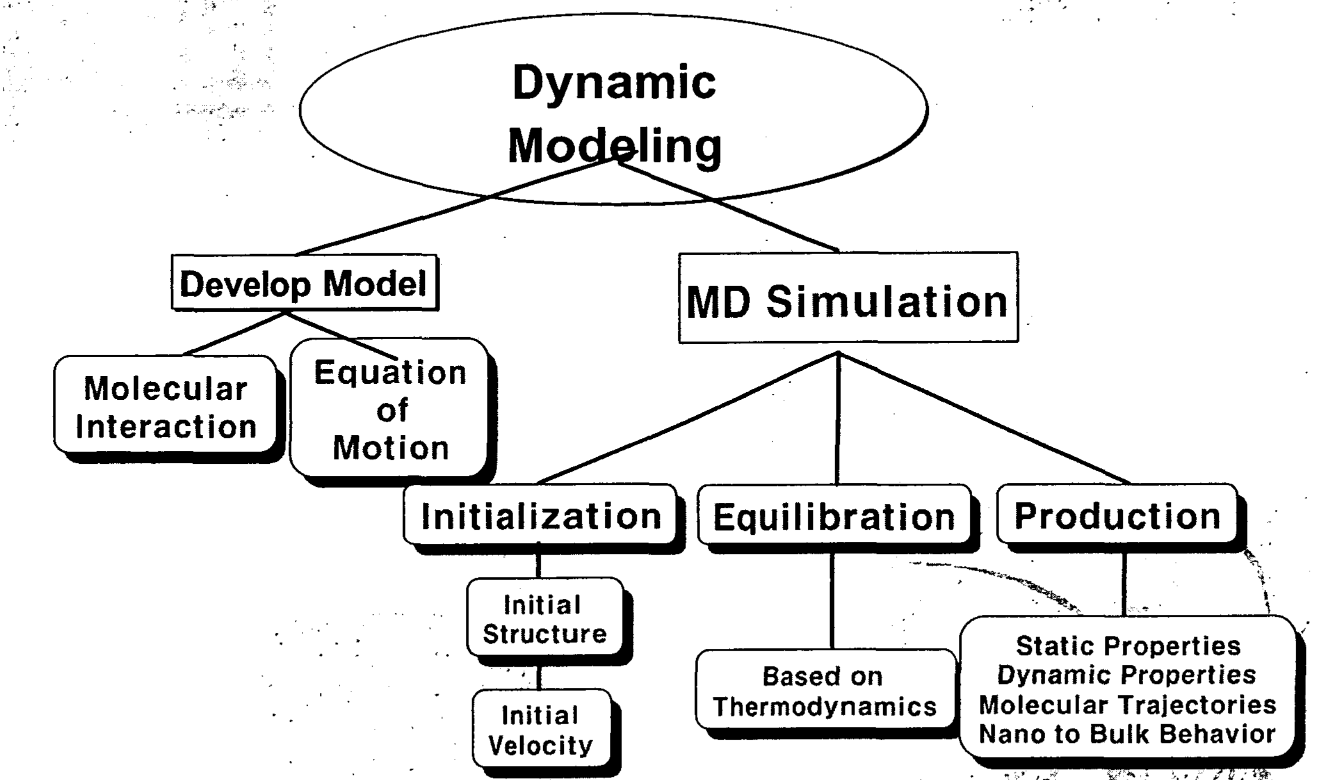
INTRODUCTION TO MD SIMULATION



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Define Initial Positions and Velocities: $\bar{r}_i(t_o)$ $\bar{v}_i(t_o)$

↓

Calculate Forces $\bar{F}_i(t_o) = -\nabla_i \Phi(\bar{r}_1, \bar{r}_2, ..., \bar{r}_N)$

↓

Solve Equations of Motions $\bar{r}_i(t_n) \Rightarrow \bar{r}_i(t_{n+1})$

$\bar{v}_i(t_n) \Rightarrow \bar{v}_i(t_{n+1})$

$t_{n+1} \Rightarrow t_n + \Delta t$

↓

Calculate Desired Physical Quantities and Trajectories

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Potentials

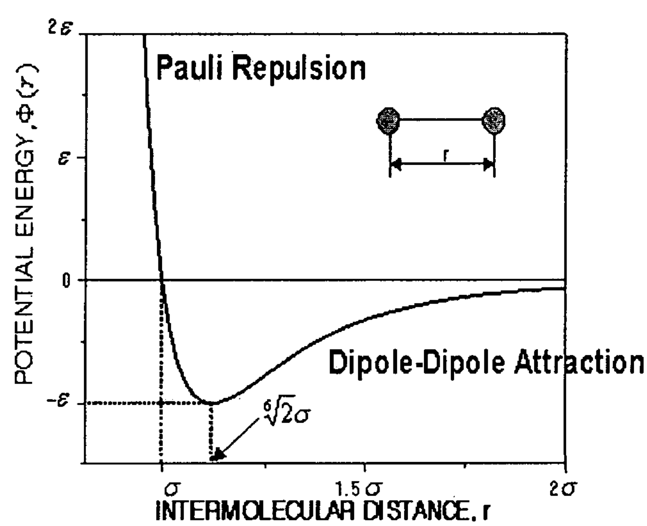
- Potential Function

$$\Phi = \sum_{i} \phi_1(\vec{r}_i) + \sum_{i}\sum_{j>i} \phi_2(\vec{r}_i, \vec{r}_j) + \sum_{i}\sum_{j>i}\sum_{k>j>i} \phi_3(\vec{r}_i, \vec{r}_j, \vec{r}_j) +$$

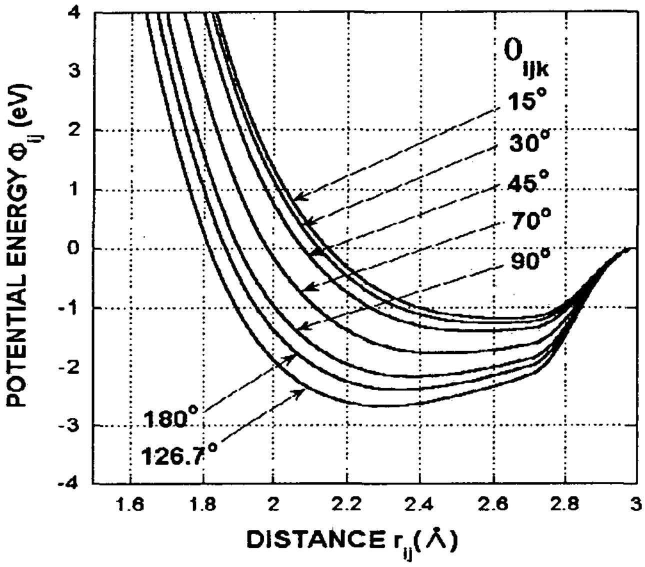
- Potential Models
  - Ne, Ar, Kr, Xe : Lennard-Jones (12-6) Pair
  - Water : ST2, SPC/E, TIP4P, CC Pair
  - Si, C : SW, Tersoff, Simplified Brenner
  - Metals : EAM, FS, SC

Lennard-Jones Potential

$$\Phi(r_{ij}) = 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - A\left(\frac{\sigma}{r_{ij}}\right)^{6}\right]$$

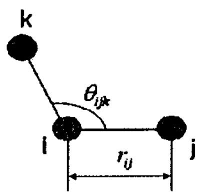


Potential Models for C and Si



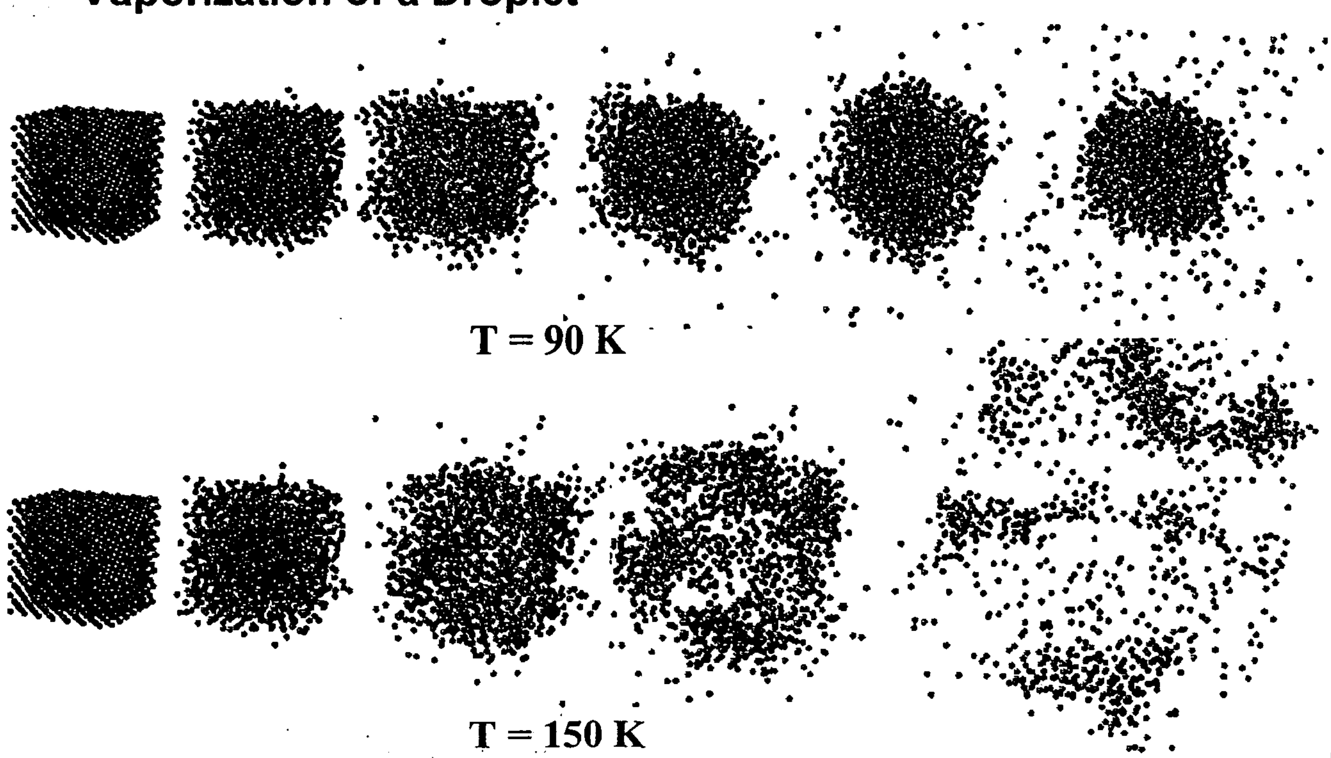
$$\Phi = \sum_i \sum_{j(i<j)} f_C(r_{ij})\{V_R(r_{ij}) - b^*_{ij} V_A(r_{ij})\}$$

$$b^*_{ij} = \frac{b_{ij} + b_{ji}}{2}, \quad b_{ij} = \left(1 + a^n \left\{ \sum_{k(\neq i,j)} f_C(r_{ik}) g(\theta_{ijk}) \right\}^n \right)^{-}$$



Visualization of Some Critical Phenomena

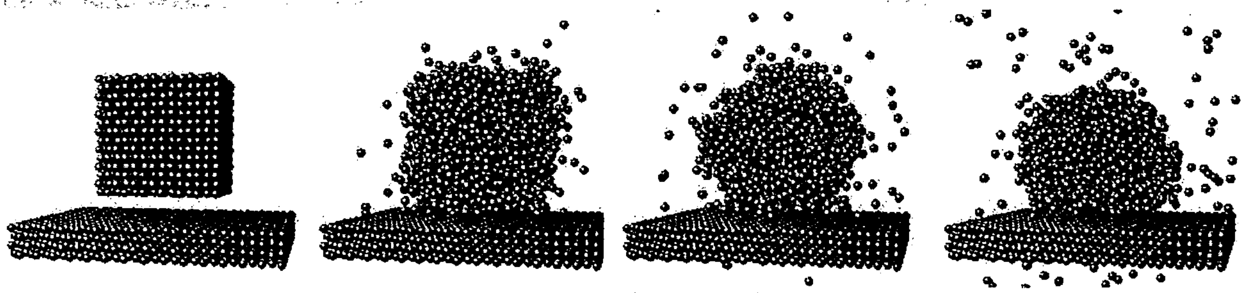
- Vaporization of a Droplet



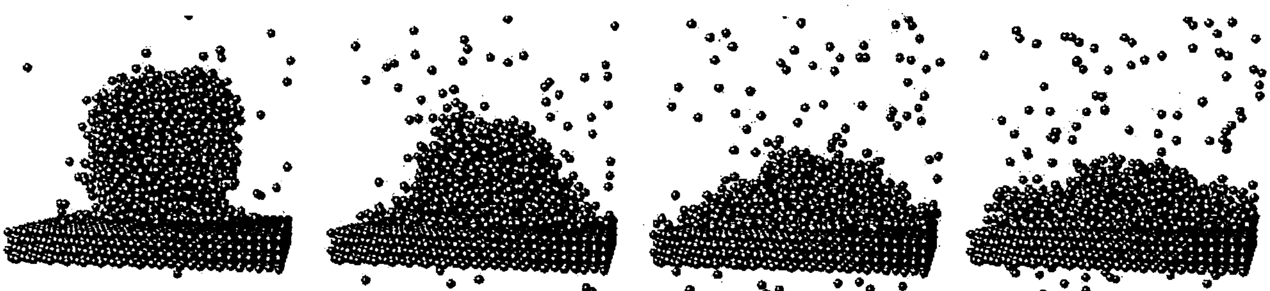
T = 90 K

T = 150 K

• Spreading of a Droplet on a Solid Surface at 90 K



Affinity Factor = 0.5



Affinity Factor = 1.0

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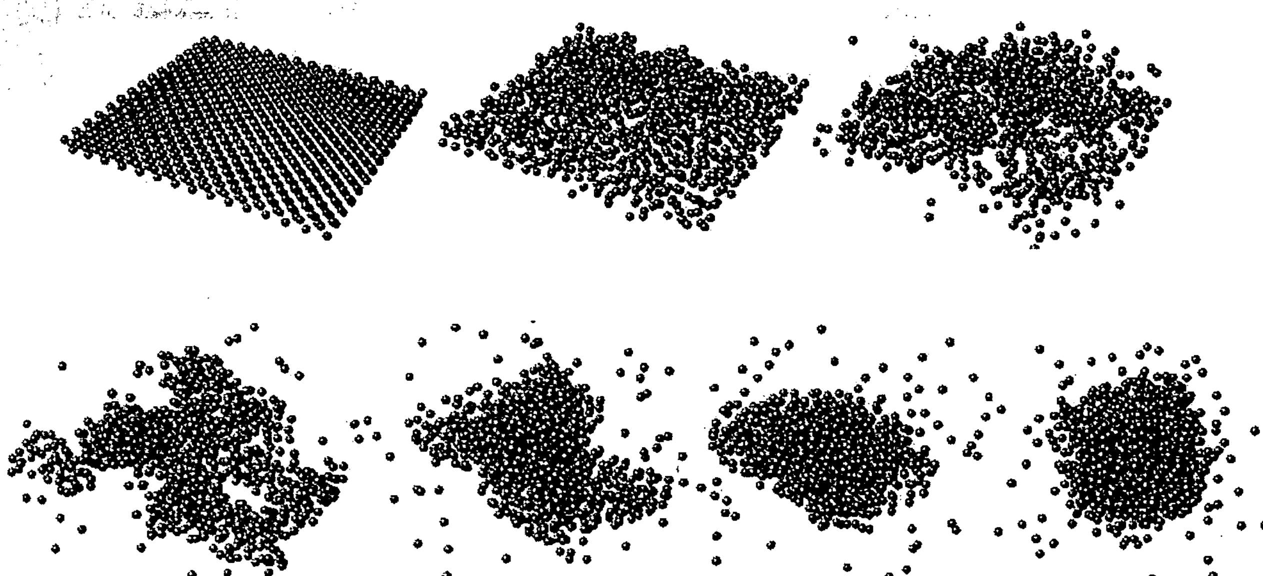
• Instability of a Liquid Thin Film at 90 K



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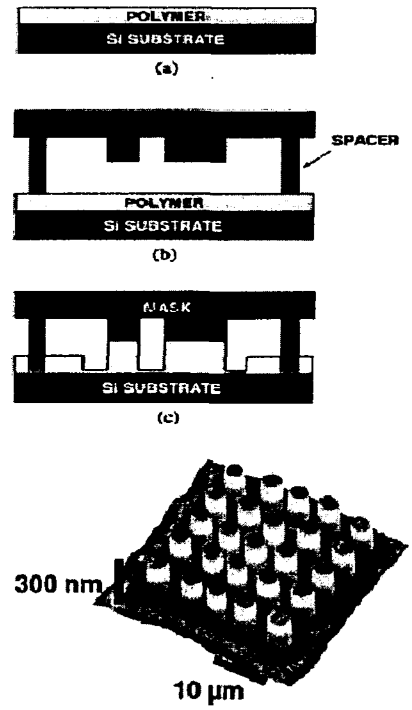
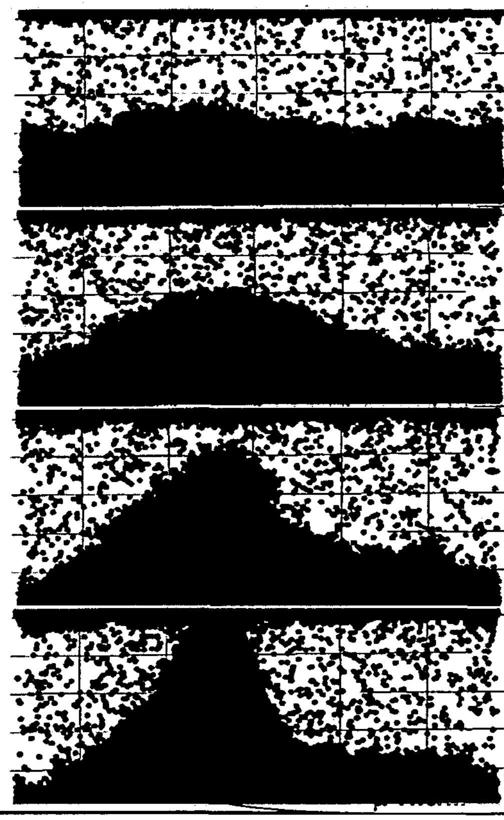
• Instability of Liquid Film on a Heated Surface

(Lithographically Induced Self-Assembly: LISA)

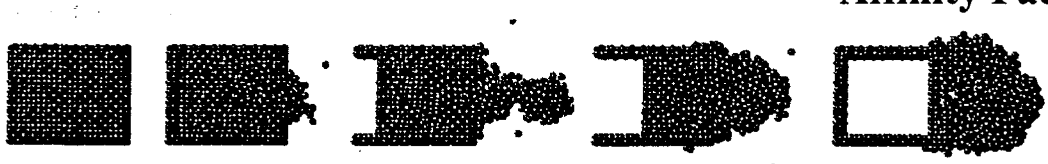


(LISA by Chou, APL, 1999)

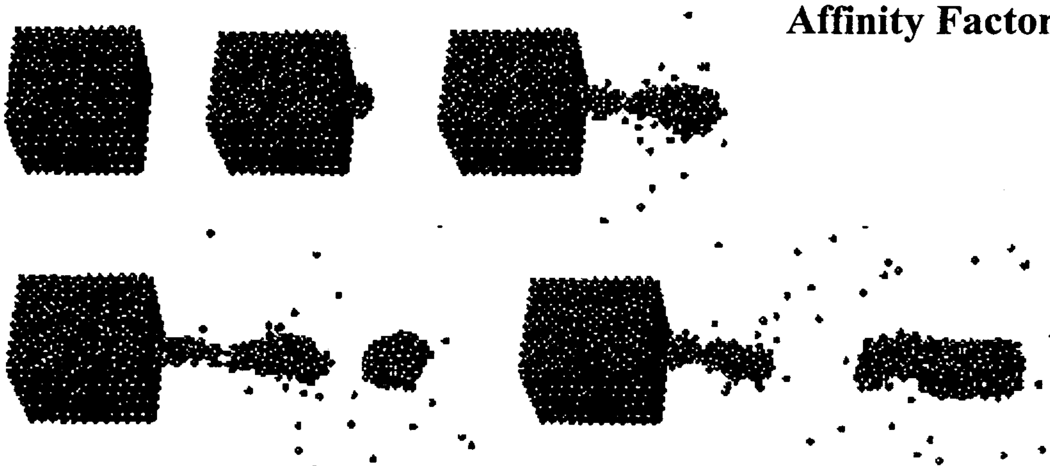


• Nanojets

Affinity Factor = 1.0



Affinity Factor = 0.1



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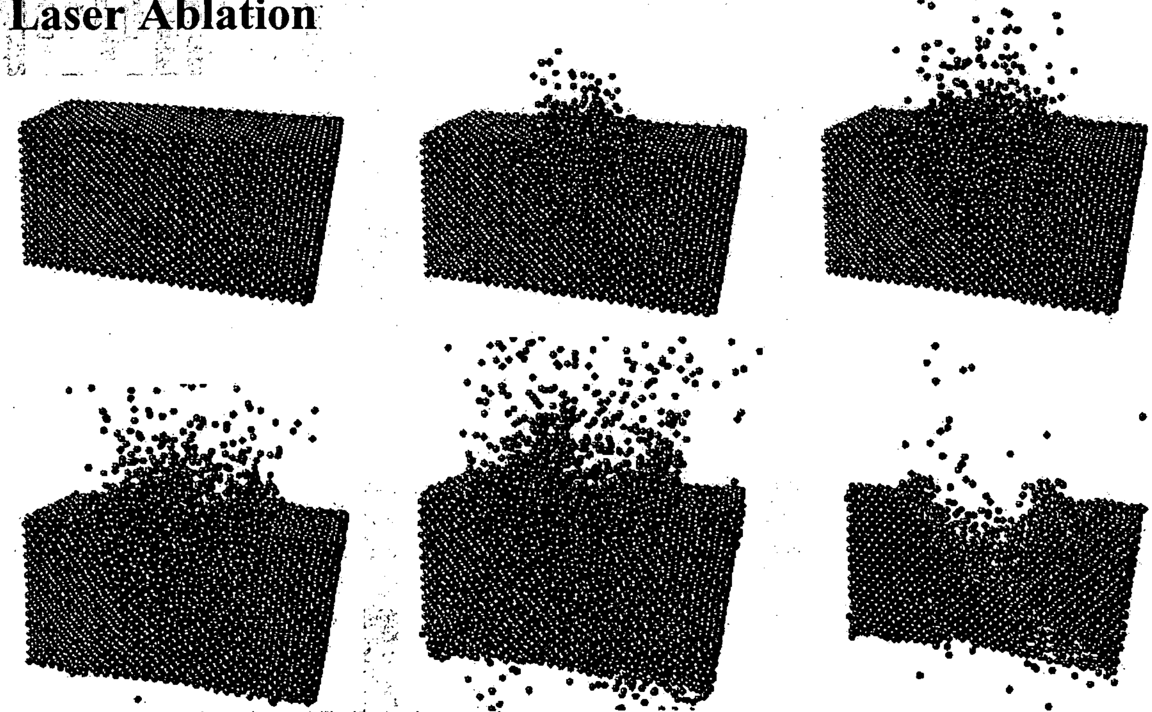
- **Laser Ablation**



Cross Sectional View

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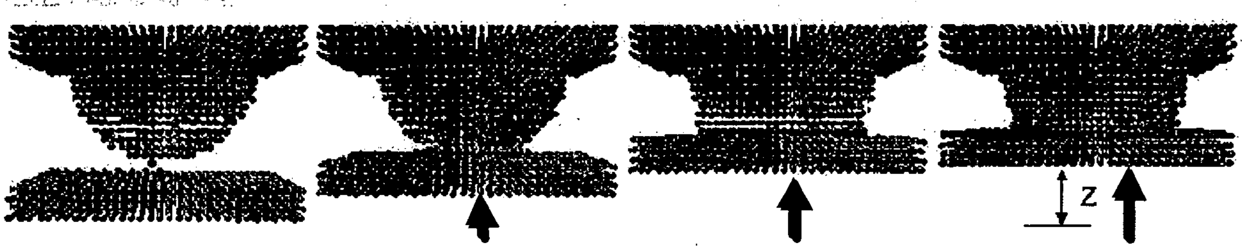
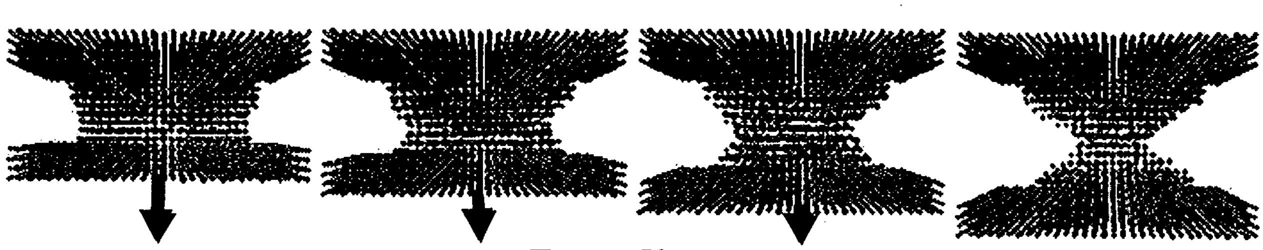
- **Adhesion and Stiction**



Approaching



Receding

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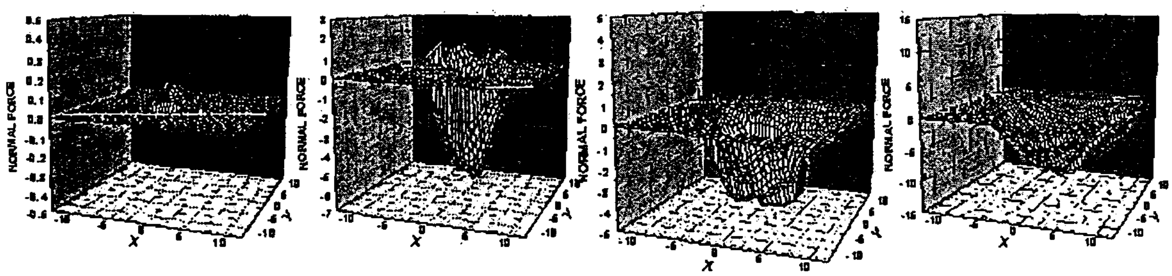
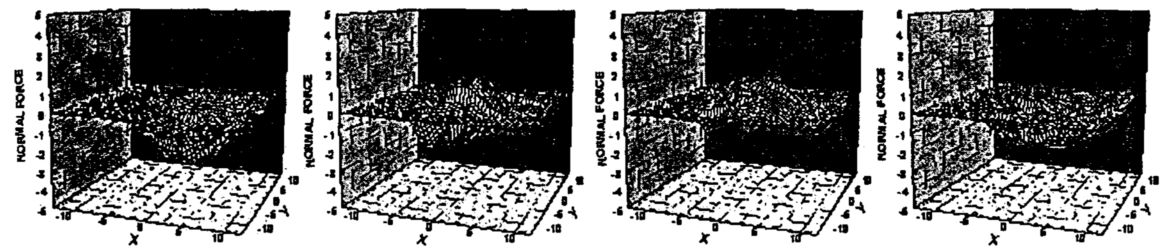
Normal Force Distribution



Z = 0.48 Z = 2.5 Z = 3.3 Z = 5.0

Approaching



Z = 4.5 Z = 3.3 Z = 1.7 Z = 0.0

Receding

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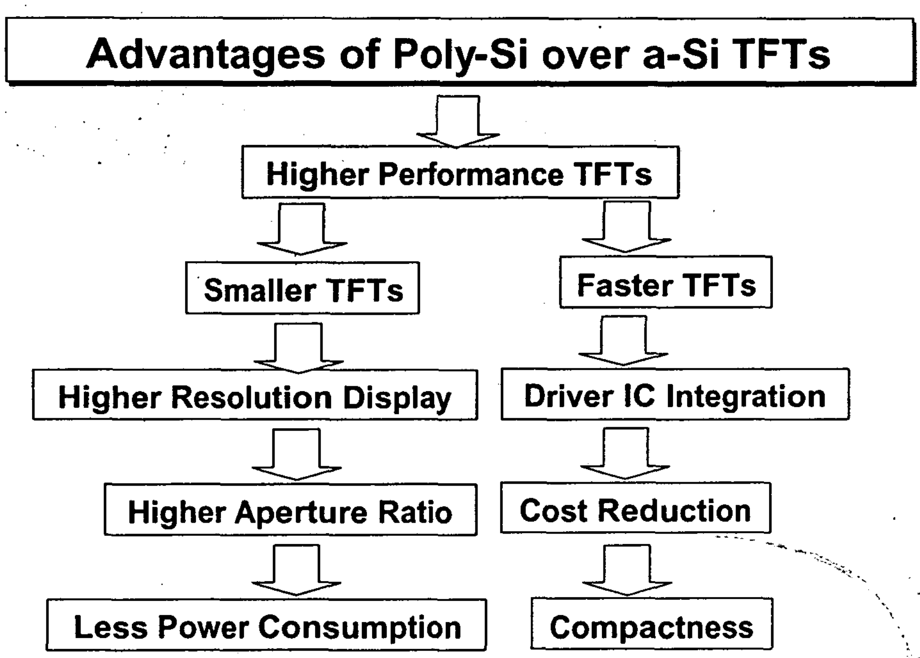
CRYSTALLIZATION OF AMORPHOUS SILICON



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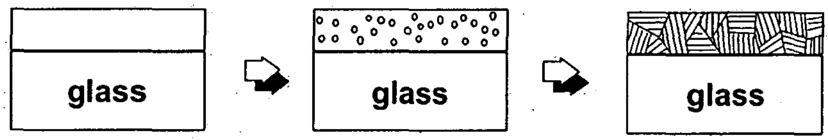
Current Technologies for Crystallization

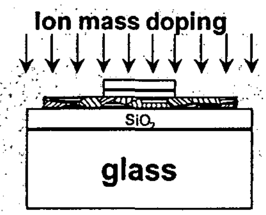
Solid-Phase Crystallization

- Low temperature crystallization of amorphous Si films



> 600C, 10 hrs

- Low temperature activation anneals for P/N ion implantation



> 600C, 3 hrs

More reliable mass-production method is needed for poly-Si TFTs on large glasses for successful poly-Si TFTs and OLEDs !

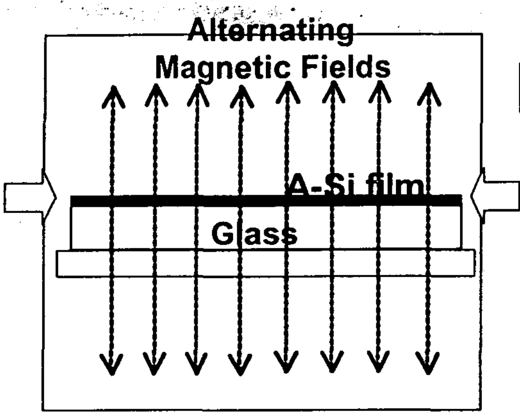
Requirements

1. Low temperature (<600°C) and short process time
2. Large process window
3. Device quality poly-Si films with an uniform structure
4. Simple and easy processes and system maintenance

<New low-temperature crystallization method>

∗ Alternating Magnetic Field Crystallization (AMFC)

Mechanisms for AMFC



Induced Electric Fields

Effects of alternating magnetic field on a-Si films

⇩

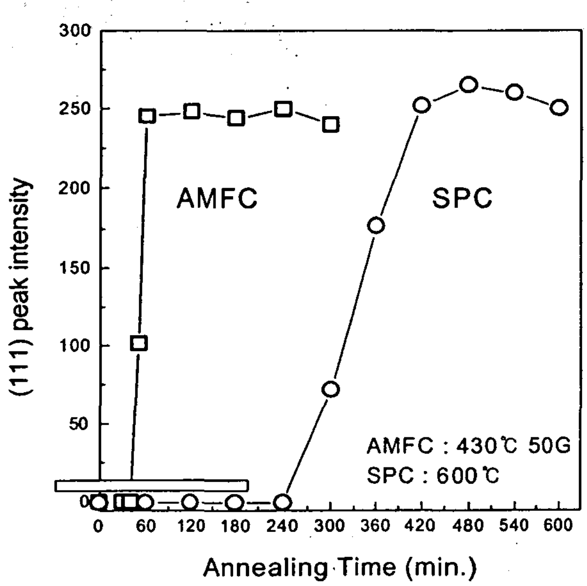
Generation of electromotive force

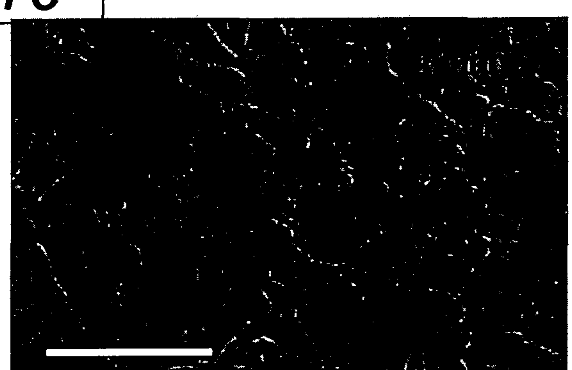
Faraday Law : EMF = $-d\Phi/dt$

⇩

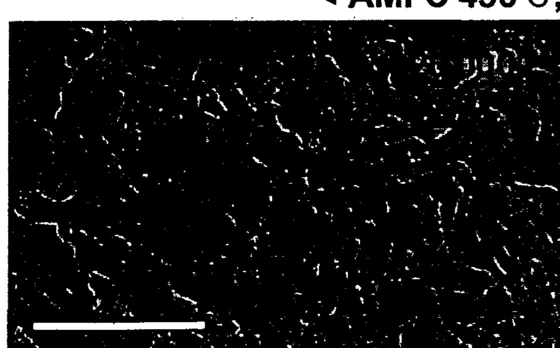
1. **Selective Joule Heating of amorphous Si films**
   Heating power = Joule Heating (EMF^2/R_{film})
2. **Field-enhanced Movement of Charged Defects**

Enhanced SPC kinetics by AMFC





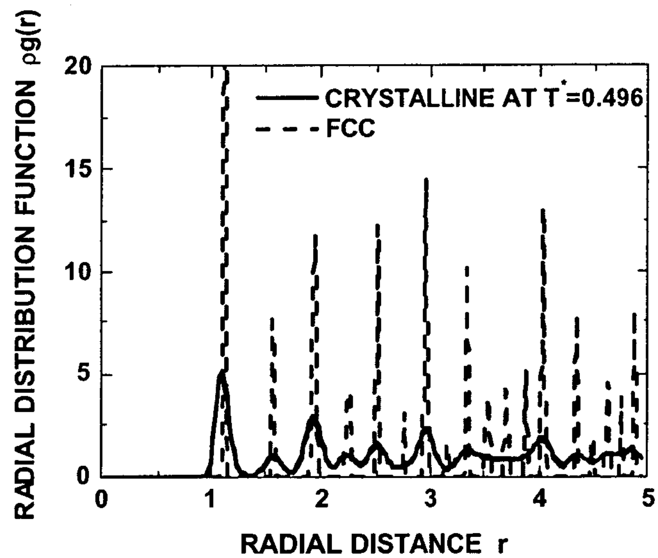
< AMFC 430℃, 1hr >

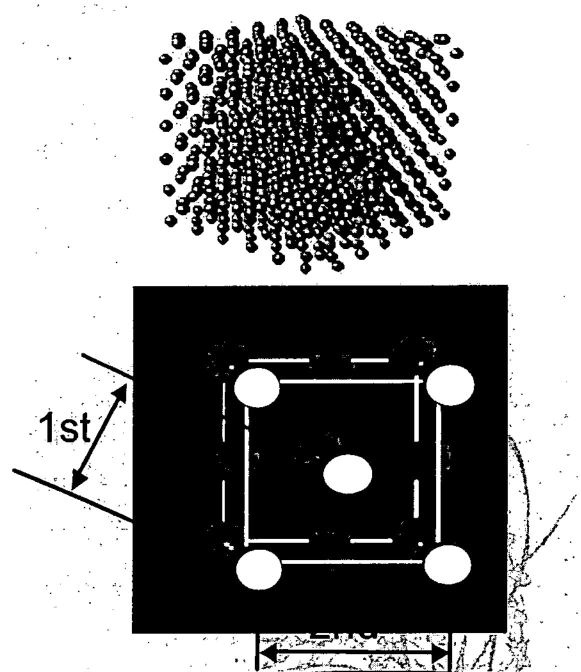


< SPC 600℃, 10hr >

Mechanism 2: External Field Induced Crystallization

MD Simulation for Crystallization of Argon





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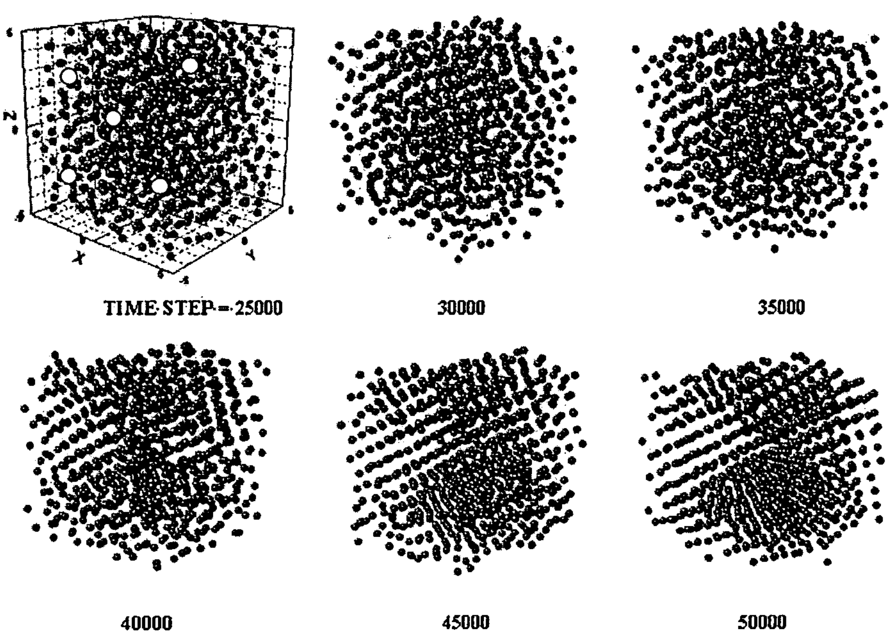
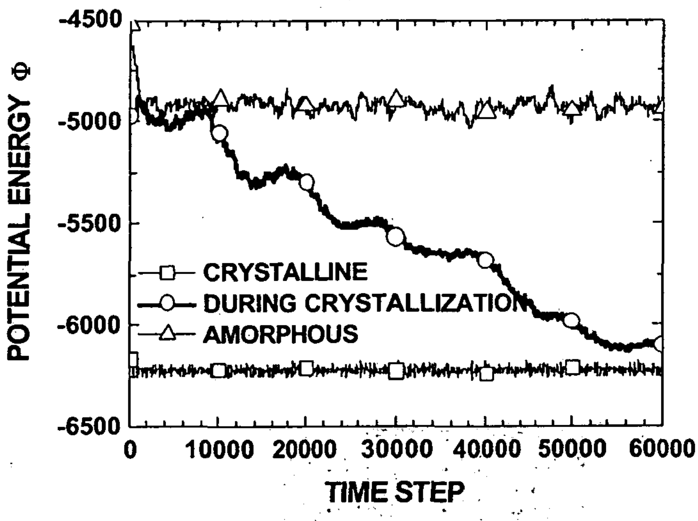
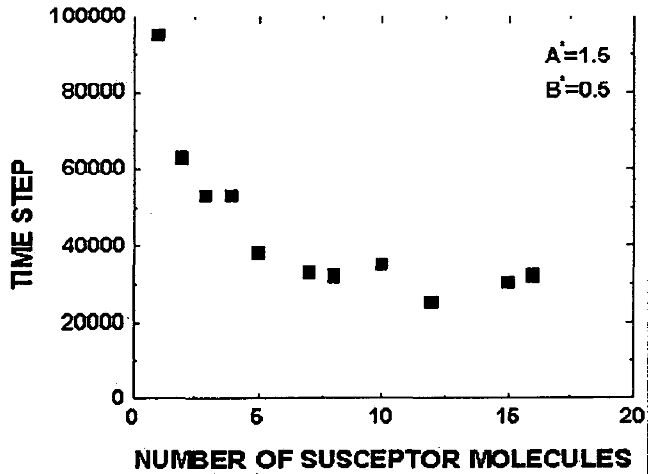
External Field Induced Crystallization of Amorphous Argon at 60 K



μ Therm

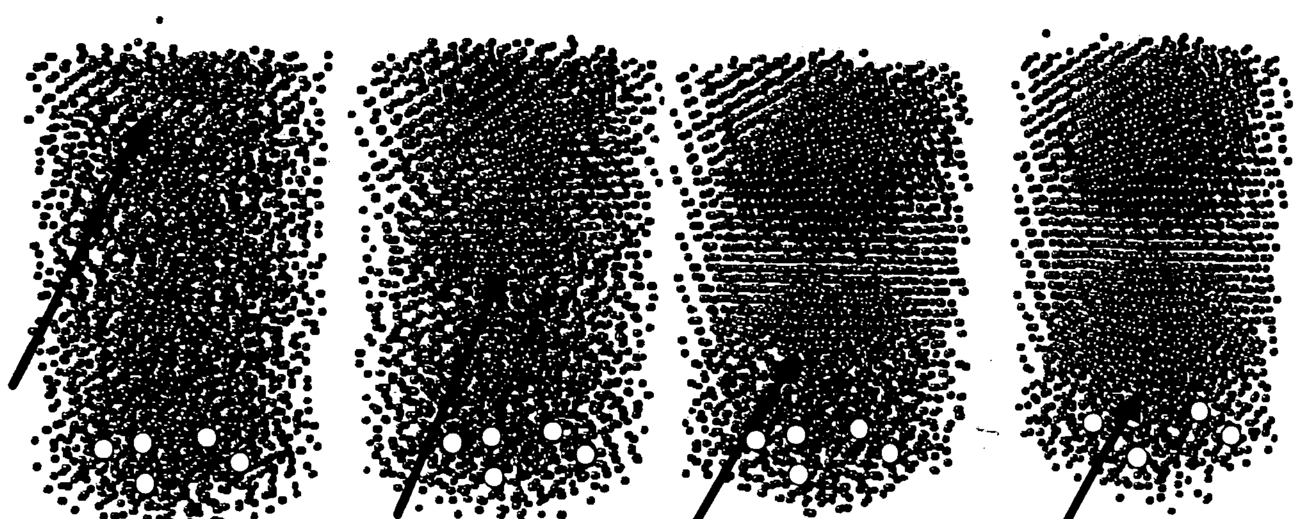
Potential Energies and Susceptor Numbers





μ *Therm*

The Growth of Crystalline Phase

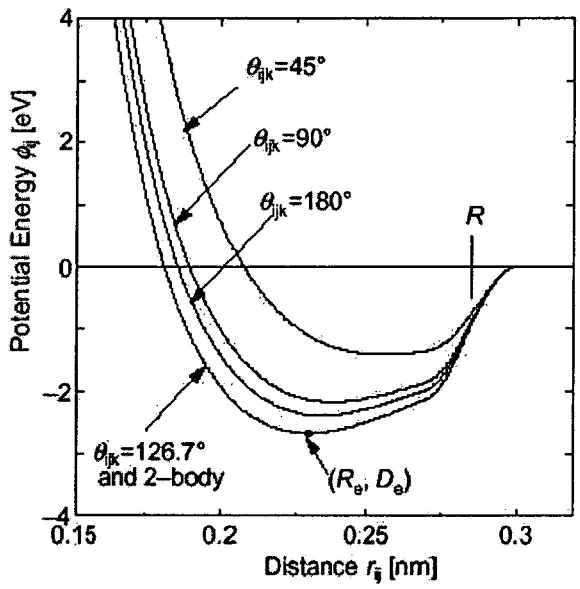


250000 280000 310000 410000

μ *Therm*

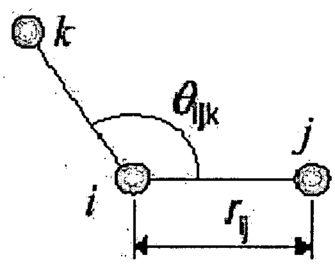
Amorphization of Si and Voronoi Analysis

MODEL: TERSOFF MULTI-BODY POTENTIAL



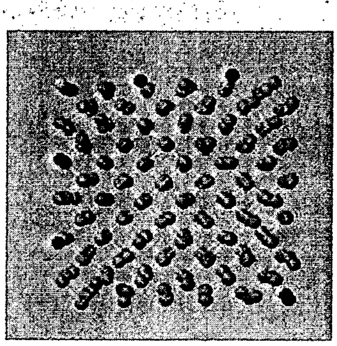
$$\Phi = \sum_i \sum_{j(i<j)} f_C(r_{ij})\left\{V_R(r_{ij}) - b^*_{ij} V_A(r_{ij})\right\}$$

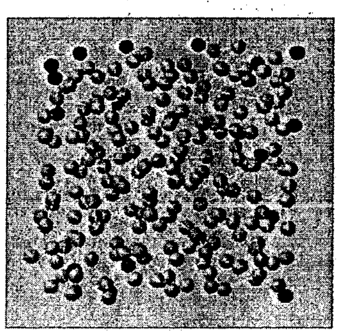
$$b^*_{ij} = \frac{b_{ij} + b_{ji}}{2}, \quad b_{ij} = \left(1 + a^n \left\{\sum_{k(\neq i,j)} f_C(r_{ik}) g(\theta_{ijk})\right\}^n\right)^{-\delta}$$

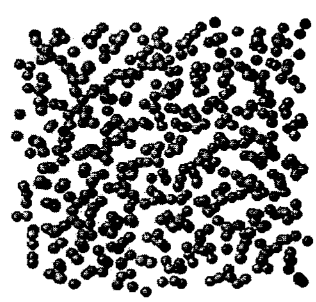


μ Therm

Amorphization of Silicon



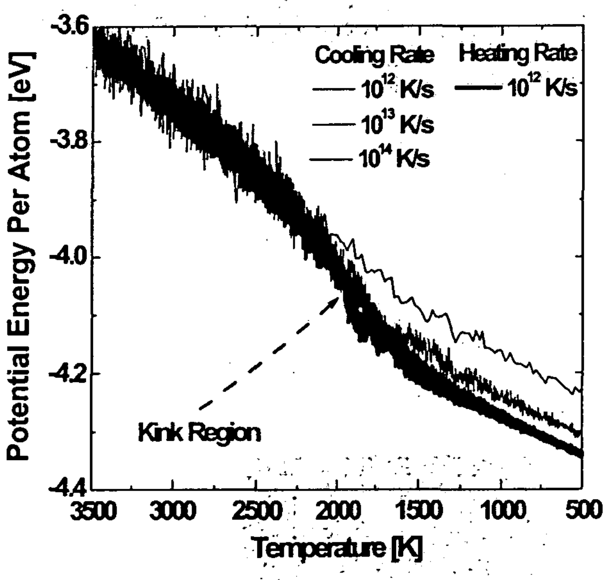




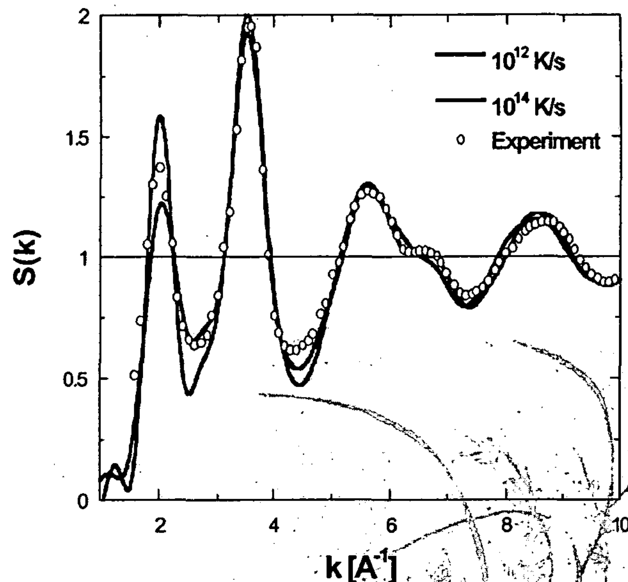
c-SI at 1000 K → LIQUID-SI at 3500 K → a-SI at 500 K

μ Therm

Potential Energy Variation during Solidification and Heating Processes



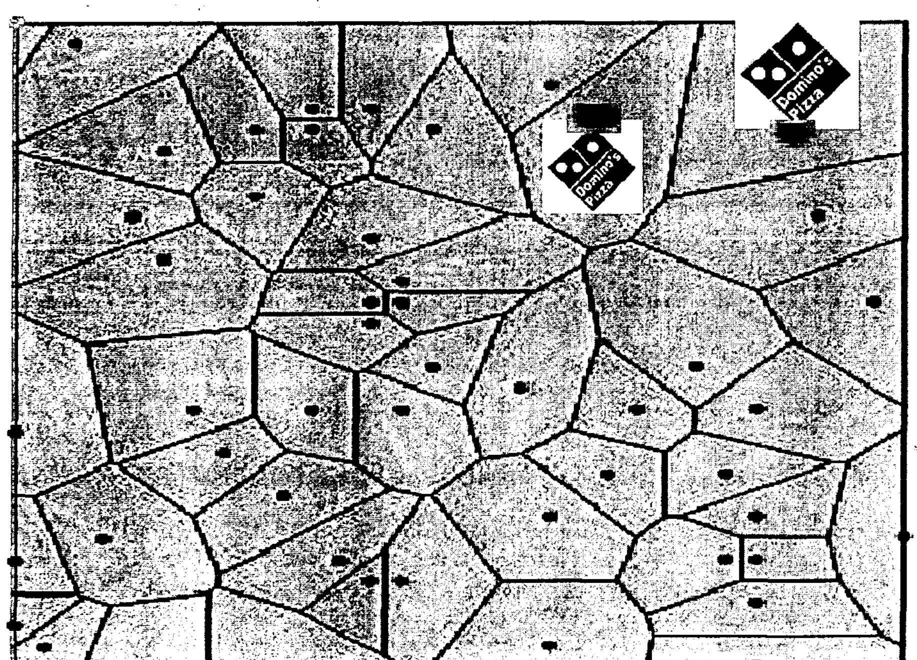
Structure Factor of a-Si at 500 K



μ Therm

Voronoi Polyhedron

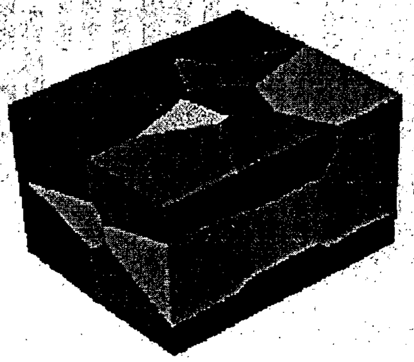
- Want to Know about Proximity to a Set of Points or Objects (Domino's Pizza)

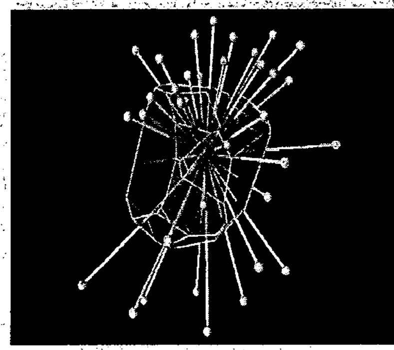


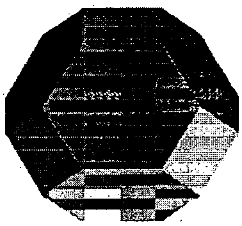
2-D VP

μ Therm

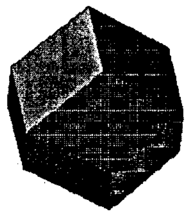
3-D VP



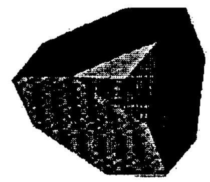




BCC



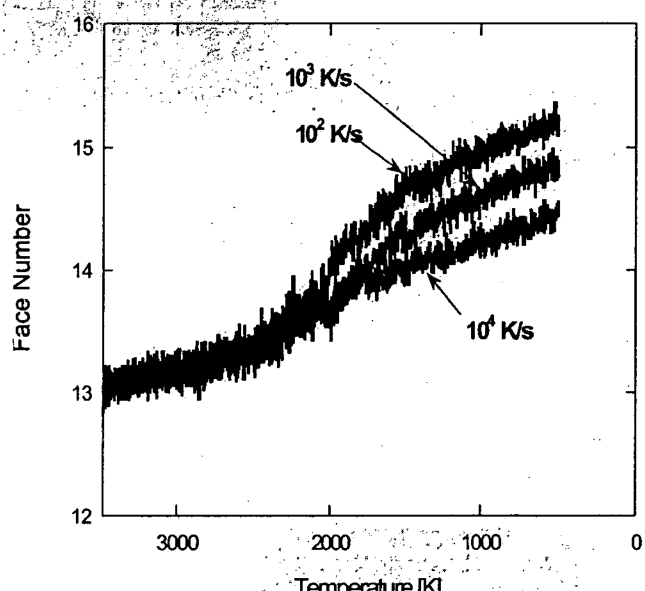
FCC



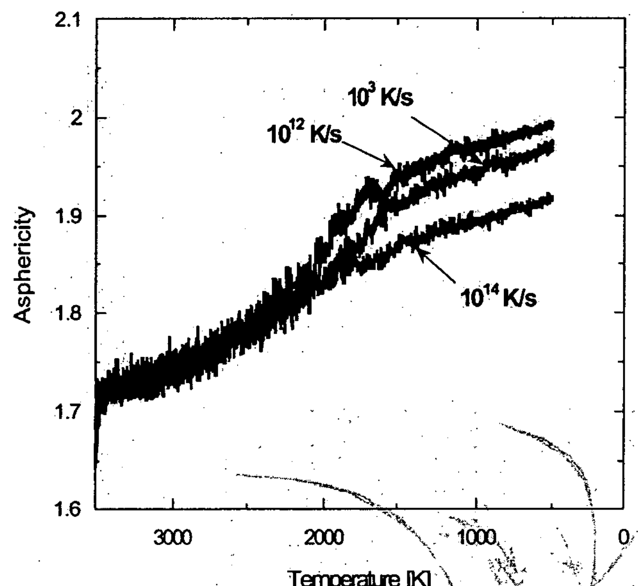
Diamond

μ *Therm*

During Solidification Process



Face Number



Asphericity

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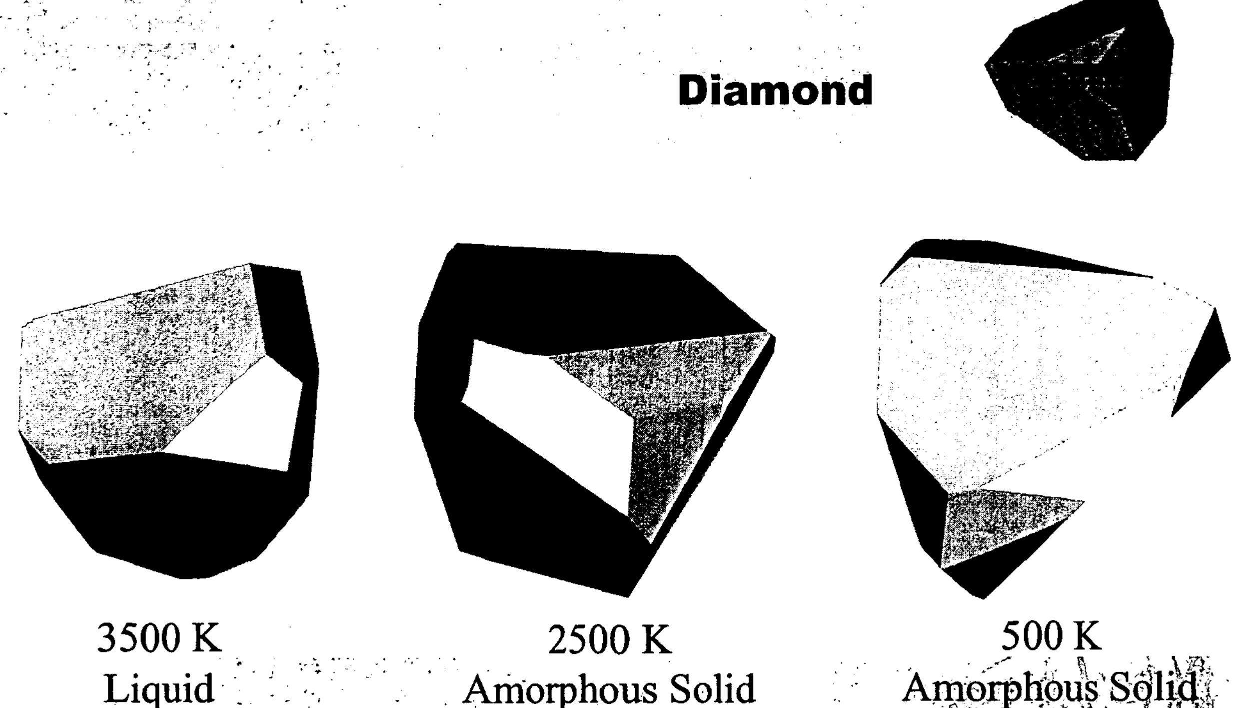
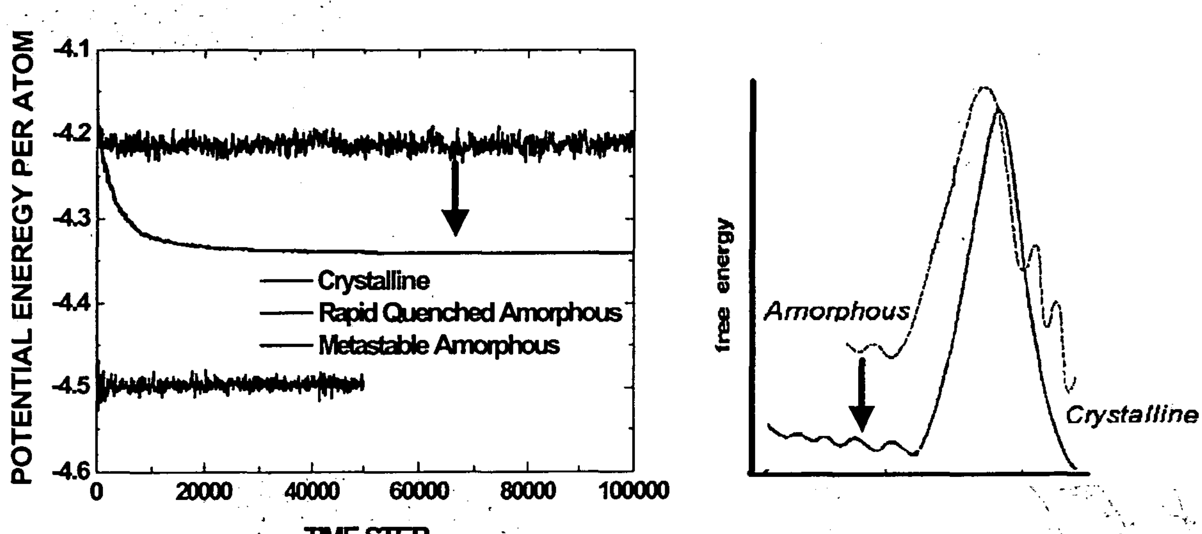
Structures of a-Si during Solidification Process



μ Therm

Homogeneous Crystallization of a-Si (Currently Unsuccessful)



POTENTIAL ENERGIES AT 1000 K

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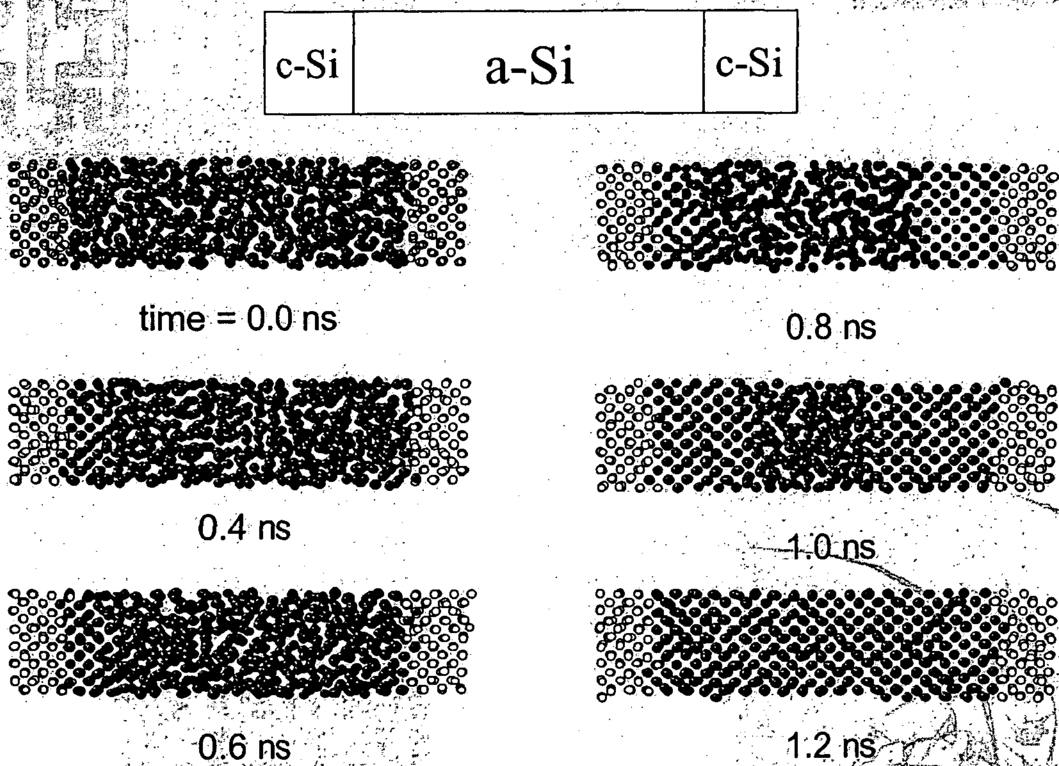
HETEROGENEOUS CRYSTALLIZATION OF a-Si



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CO-RESEARCHERS

- Y.K. Choi (Chung-Ang University)
- O.M. Kwon (Korea University)
- H.J. Kim (Hongik University)
- M.S. Han (Seoul National University, Post-Doc)
- S.H. Lee (Seoul National University, Post-Doc)
- B.S. Lee (Seoul National University, Graduate Student)
- D.B. Lee (Seoul National University, Graduate Student)
- B.K. Kim (Seoul National University, Graduate Student)
- J.H. Park (Hongik University, Graduate Student)
- C.H. Yoon (Hongik University, Graduate Student)

μ *Therm*

CONCLUDING REMARKS

- MD can describe various nano-scale critical phenomena such as vaporization/formation/spreading of a droplet, instability of liquid thin films and LISA process, nanojets, laser ablation, adhesion and stiction.
- Voronoi analysis proves that structural change occurs during the solidification process of liquid silicon.
- MD simulation for a-Si shows that heterogeneous nucleation can be expedited significantly by external fields, while homogeneous nucleation is impossible.

μ Therm