

Radiative Heat Transfer in Fractal Structures

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613. WE-Heraeus-Seminar on
“Heat Transfer and Heat Conduction on the Nanoscale”

Overview

- Radiative Heat Transfer in Many-body Systems.
- Why Fractals?
- Cluster-Cluster Aggregation.
- Overlapping Dipole Model.
- Results: Self and Mutual conductance, Tip-Fractal HE

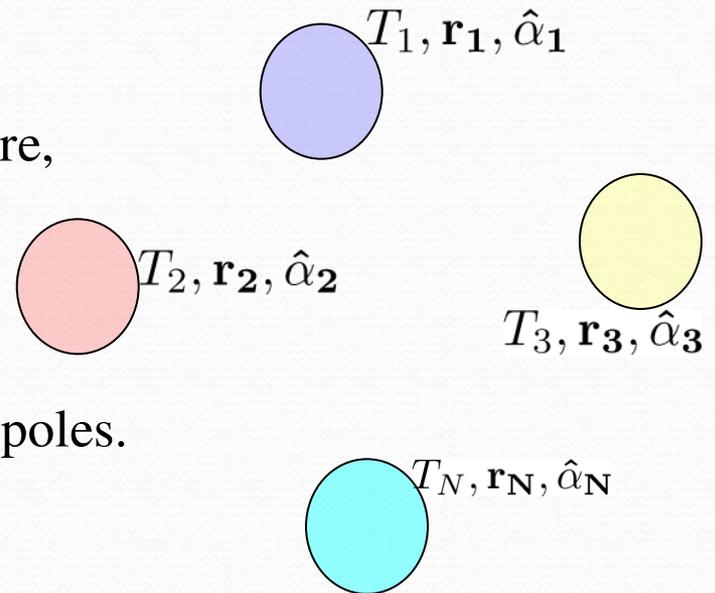
Heat flow in many-body systems

□ System consists N nanoparticles.

□ Each nanoparticle characterizes by its Temperature, Position and Polarizability Tensor.

□ Nanoparticles are approximated by fluctuating dipoles.

□ Nanoparticles exchange energy through dipole interactions.



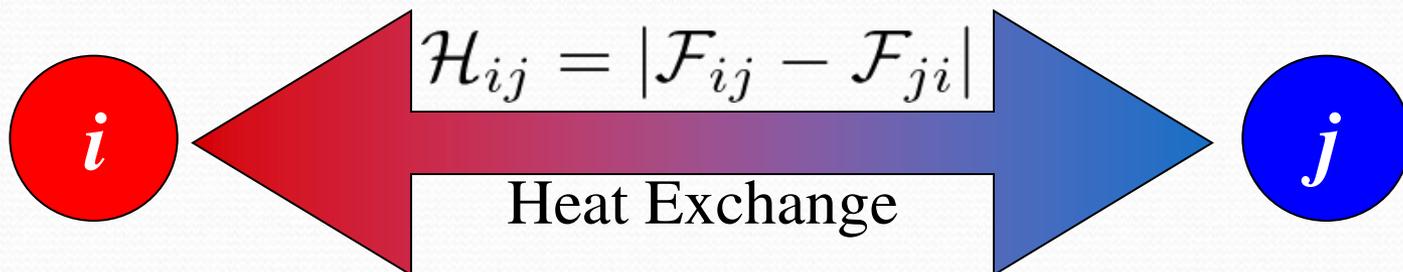
Heat flow in many-body systems

Power dissipated in i-th nanoparticle → Particle will heat up or cools down

$$\mathcal{P}_i = \langle \mathbf{E}_i^*(t) \cdot \dot{\mathbf{P}}_i(t) \rangle = 2 \int_0^\infty \omega \frac{d\omega}{4\pi^2} \text{Im}[\langle \mathbf{E}_i^*(\omega) \cdot \mathbf{P}_i(\omega) \rangle].$$

$$\mathcal{P}_i = \mathcal{F}_i(T_i) + \sum_{j \neq i} \mathcal{F}_{i,j}(T_j)$$

- LOSE ENERGY: Cooling of each particle due to its radiation.
- GAIN ENERGY: Direct and indirect heating of each particle by the others.



Transitions probability - Conductance

$$\mathcal{F}_i = \int_0^\infty \frac{d\omega}{2\pi} \mathcal{T}_{ii}(\omega) \Theta(\omega)$$

$$\mathcal{T}_{ii} = 2\text{ImTr}[\hat{\mathbf{A}}_{ii} \text{Im}(\hat{\chi}_i) \hat{\mathbf{C}}_{ii}^\dagger]$$

Self Conductance

$$\mathcal{G}_i(T) \equiv \frac{\partial \mathcal{F}_i}{\partial T}$$

$$\mathcal{H}_{ij} = \int_0^\infty \frac{d\omega}{2\pi} \mathcal{T}_{ij}(\omega) \Delta\Theta(\omega)$$

$$\mathcal{T}_{ij} = 2\text{ImTr}[\hat{\mathbf{A}}_{ij} \text{Im}(\hat{\chi}_j) \hat{\mathbf{C}}_{ij}^\dagger]$$

Mutual Conductance

$$\mathcal{G}_{ij}(T) \equiv \frac{\partial \mathcal{H}_{ij}}{\partial T}$$

\mathbf{A} and \mathbf{C} depends on dyadic green functions

χ is the susceptibility tensor

Heat Transfer Probability

Two-Body System

$$\mathcal{T}_{12}^{2-body}(\omega) = 2K^4 \text{Tr} \left(\hat{\mathcal{M}} \hat{\mathbf{G}}_{12} \hat{\mathcal{M}}^\dagger \hat{\mathbf{G}}_{12}^\dagger \text{Im} \hat{\chi}^{(1)} \text{Im} \hat{\chi}^{(2)} \right)$$

$$\mathcal{M}^{-1} = \left(\hat{\mathbf{1}} - K^4 \hat{\alpha}^{(1)} \hat{\mathbf{G}}_{12} \hat{\alpha}^{(2)} \hat{\mathbf{G}}_{12} \right)$$



Polarizability Tensor

Shape, Size, Orientation, Material, Environment

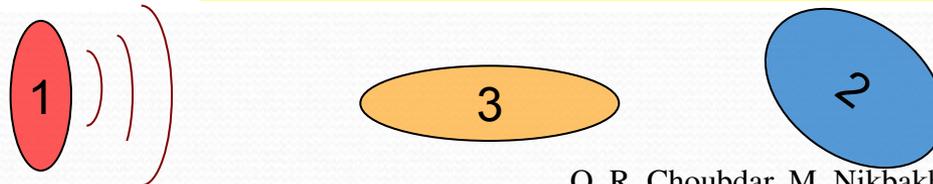
Dyadic Green Tensor

Separation distance
Geometrical Arrangement

Three-Body System

$$\mathcal{T}_{12}(\omega) = 2K^4 \text{Tr} \left\{ \left(\hat{\mathbf{G}}_{12} \hat{\mathbf{G}}_{12}^\dagger + 2K^2 \text{Re} \left(\hat{\mathbf{G}}_{12}^\dagger \hat{\mathbf{G}}_{13} \hat{\mathbf{G}}_{23} \hat{\alpha}_3 \right) + K^4 \hat{\mathbf{G}}_{13}^\dagger \hat{\mathbf{G}}_{13} \hat{\mathbf{G}}_{23}^\dagger \hat{\mathbf{G}}_{23} \hat{\alpha}_3 \hat{\alpha}_3^\dagger \right) \times \left(\hat{\mathcal{M}} \hat{\mathcal{M}}^\dagger \text{Im} \hat{\chi}^{(1)} \text{Im} \hat{\chi}^{(2)} \right) \right\}$$

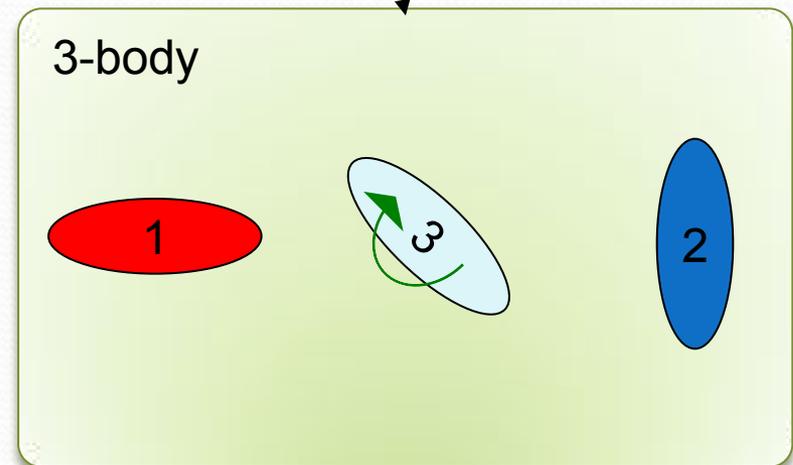
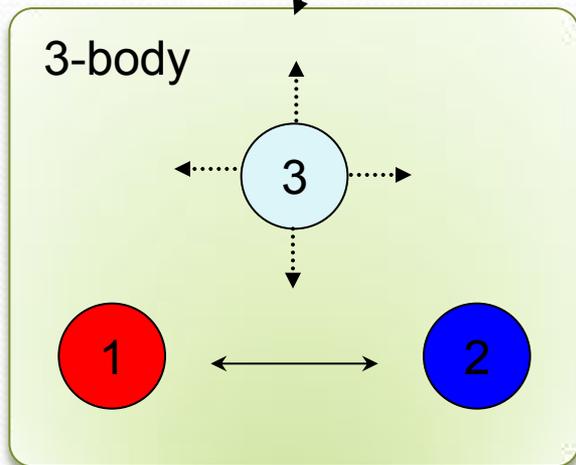
$$\mathcal{M}^{-1} = \left(\hat{\mathbf{1}} - K^4 \hat{\alpha}^{(1)} \hat{\mathbf{G}}_{12} \hat{\alpha}^{(2)} \hat{\mathbf{G}}_{12} - K^4 \hat{\alpha}^{(1)} \hat{\mathbf{G}}_{13} \hat{\alpha}^{(3)} \hat{\mathbf{G}}_{13} - K^4 \hat{\alpha}^{(2)} \hat{\mathbf{G}}_{23} \hat{\alpha}^{(3)} \hat{\mathbf{G}}_{23} - 2K^6 \hat{\alpha}^{(1)} \hat{\mathbf{G}}_{12} \hat{\alpha}^{(2)} \hat{\mathbf{G}}_{23} \hat{\alpha}^{(3)} \hat{\mathbf{G}}_{13} \right)$$



Many-Body Effect

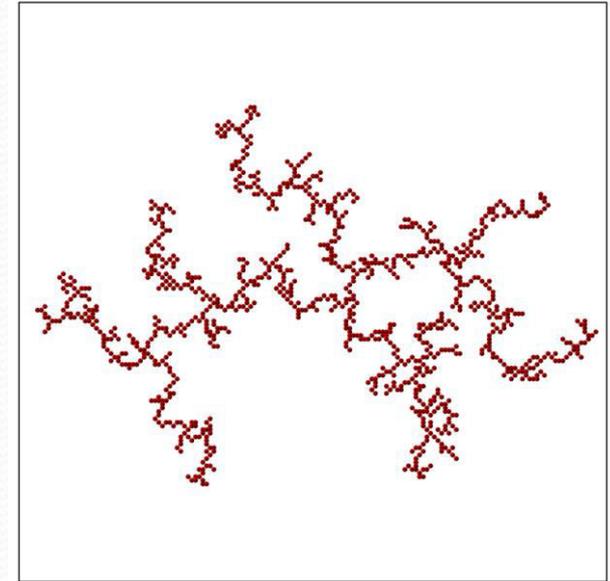
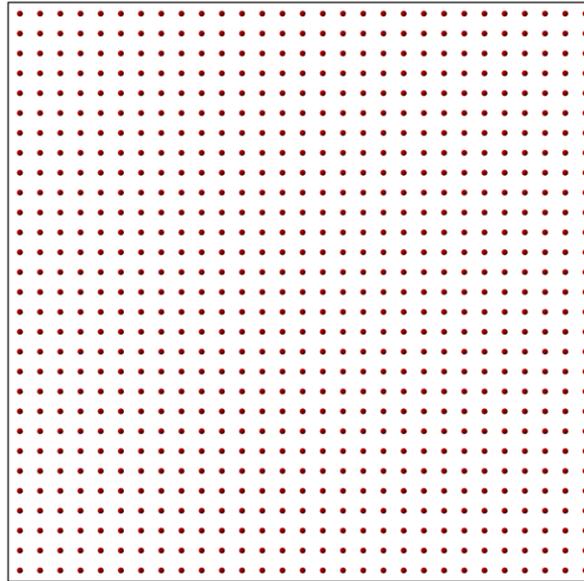
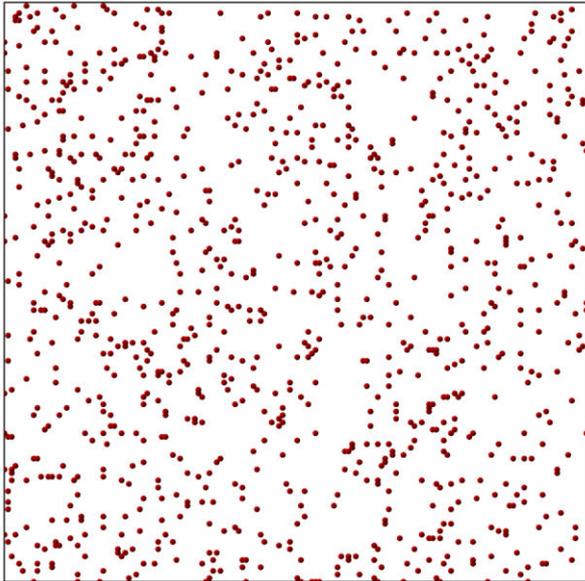
Increasing the number of particles:

- Radiating field scattered many times between nanoparticles.
- Geometrical arrangement and Shape, size, relative orientation and material



P. Ben-Abdallah, *et. al*, Phys. Rev. Lett., **107**, 114301 (2011)
R. Messina, *et. al*, Phys. Rev. B, **88**, 104307 (2013)
M. Nikbakht. J. Appl. Phys. **116**, 094307 (2014)
M. Nikbakht. Eur. Phys. Lett. **110**, 1004 (2015)
P. Ben-Abdallah. *et. al*. **107**, 053109 (2015)
Y. Wang. *et. al*, AIP. Adv. **6**, 025104 (2016)
O. R. Choubdar, M. Nikbakht. J. Appl. Phys, **120**, 144303(2016)

Why Fractals?



Disordered

Non-Fractal

Ordered

Fractal

- ✓ Translational invariance
- ✓ Transmit running waves
- ✓ Nanoparticles have a similar feeling

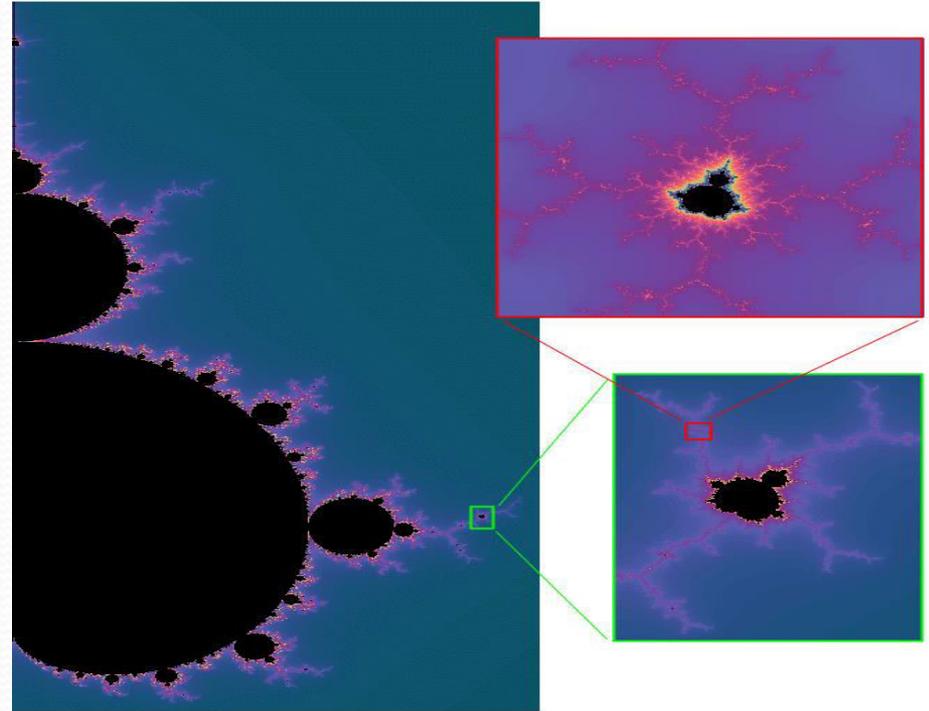
- ✓ Scale invariance
- ✓ Can NOT Transmit running waves
- ✓ Good candidates for heat localization

Common features of fractals

- Self Similar (Scale invariant)
- Something “feels the same”
regardless of scale

- Fractal Dimension

Introduced by Mandelbort (1977)



D_f : Fractal Dimension \rightarrow Non-integer Number

D : Embedding Space \rightarrow Integer Number

$$D_f \leq D$$

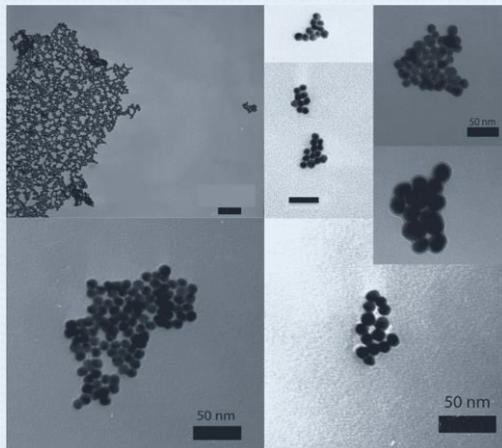
Fractal Aggregated Nano-particles

Aggregation of colloidal nanoparticle in a solutions

1. Suspension of nanoparticle → Experimental methods
2. Assembly of nanoparticles
 - Chemical methods
 - Electro-chemical method
 - High power Laser-Matter interaction
3. 3D-fractal aggregation
4. Deposition to form 2D-fractal

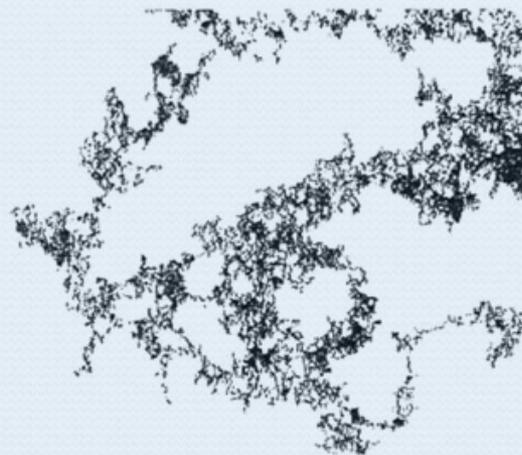
2D-Fractal

Au nanoparticle cluster



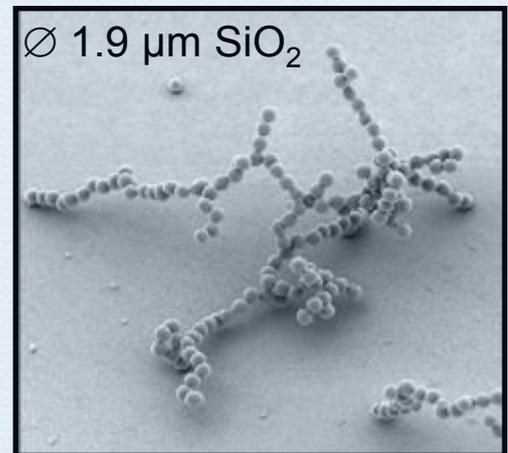
Clark et al. 2015

Ag fractal aggregate



Shalaev et al. 2006

3D-Fractal



Blum et al. 1998

Cluster-Cluster Aggregation (CCA)

Random distribution of Nanoparticles

Peak a nanoparticle (or sub-cluster) in random

Random movement
(periodic boundary condition)

Stick upon collision
Formation of sub-cluster

Large Cluster Formation

**Simple
Cluster Cluster Aggregation**

by

Moladad Nikbakht

Mohammad H. Mahdieh

Grid size: 300

Number of Particles: 9000



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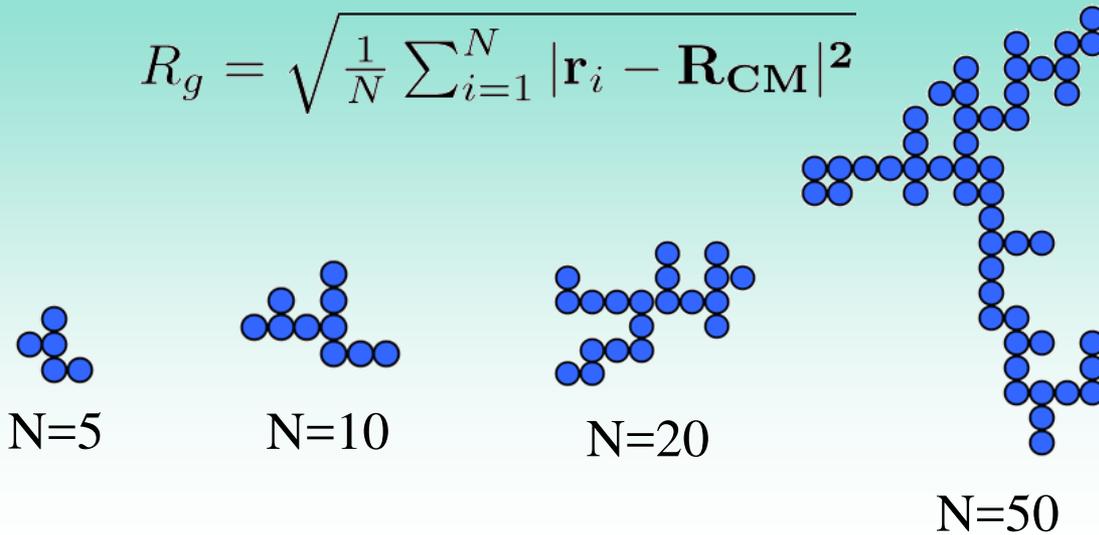
- ✓ Introduced by Meakin and Kolb (1983)
- ✓ Process is similar for CCA in 3-dimension

M. Nikbakht, *et. al*, J. Phys. Chem. C. **115**, 1561 (2011)

Fractal Dimension: D_f

Number of nanoparticles vs Gyration radius

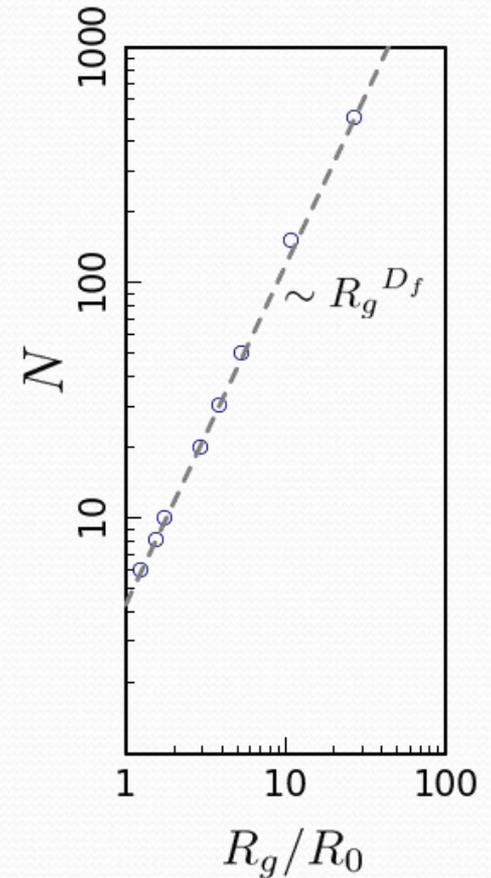
$$R_g = \sqrt{\frac{1}{N} \sum_{i=1}^N |\mathbf{r}_i - \mathbf{R}_{\text{CM}}|^2}$$



2D-CCA $D = 2$ $D_f \simeq 1.44$

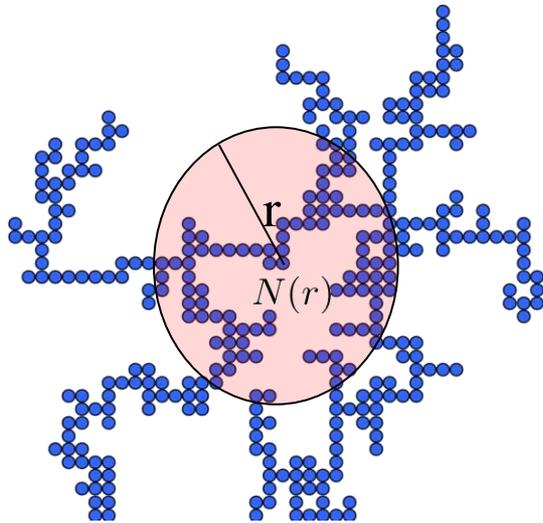
3D-CCA $D = 3$ $D_f \simeq 1.78$

$D_f = D$ for ordered and disordered structures



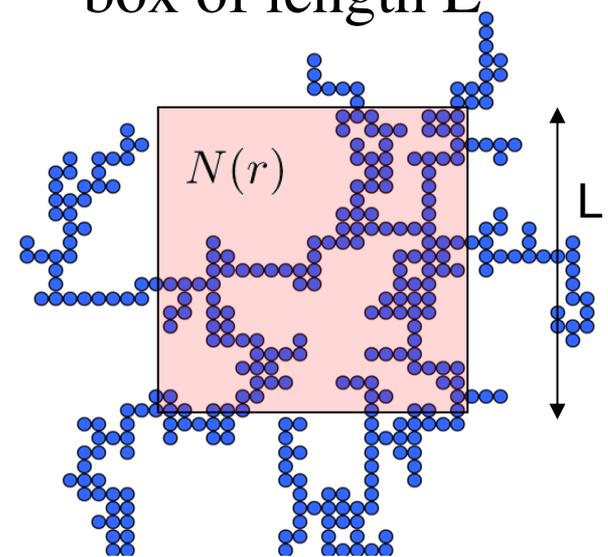
$$N \sim \langle R_g \rangle^{D_f}$$

Number of neighbors within a sphere of radius r



$$N(r) \sim r^{D_f}$$

Number of neighbors within a box of length L

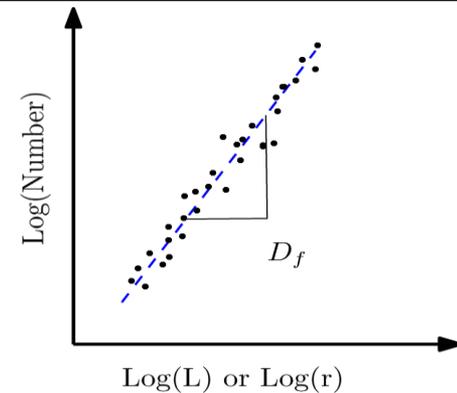


$$N(L) \sim L^{D_f}$$

2D-CCA $D = 2$ $D_f \simeq 1.44$

3D-CCA $D = 3$ $D_f \simeq 1.78$

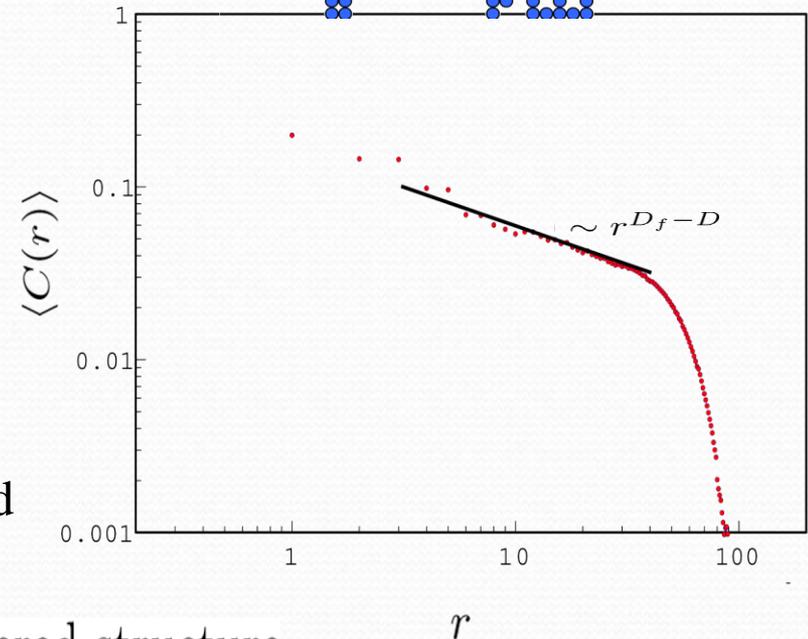
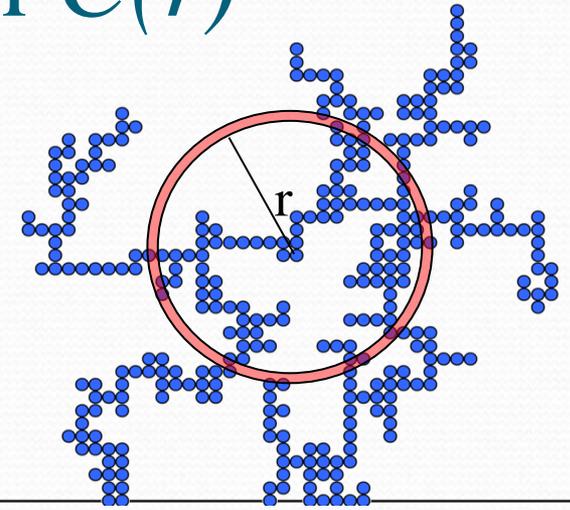
$D_f = D$ for ordered and disordered structures



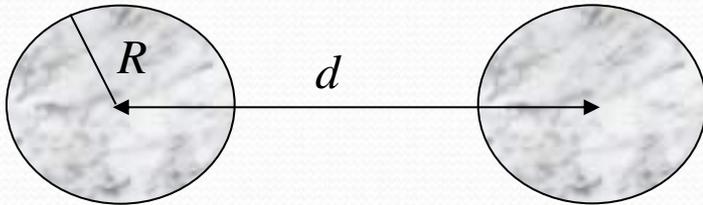
Density Correlation function $C(r)$

- ✓ Related to the probability of finding a nanoparticle at distance r from a given nanoparticle $C(r) \sim r^{D_f - D}$
- ✓ High probability of finding some particles in close proximity of each particle in fractal aggregates, accounts for strong interparticle interaction.
- ✓ The volume fraction filled by the particles is very small (tends to zero for large N).
- ✓ Rapid decrease in the correlation for large separation distance.
- ✓ The averaging is done for nanoparticles around the CM and then over several samples.

$C(r) = \text{Constant}$, $D_f = D$, for ordered and disordered structure



Touching Nano-particles



Dipole Approximation

Small Radius

Large Separation



Radiation field of the fluctuating dipole is not homogeneous inside the adjacent particle.

- Take into account the multipole moments contribution to the heat transfer

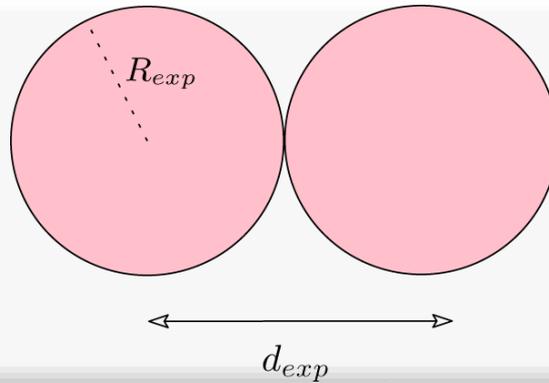
A. Perez-Madrid, et. al (2008), ...

- **Molecular dynamics simulation** G. Domingues, et. al (2005), ...

- **Overlapping Dipole Model** (E. M. Purcell 1973, V. A. Markel 1996)

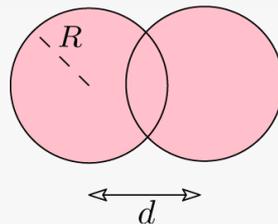
Overlapping Dipole Model

Experiment



$$d_{exp}/R_{exp} = 2$$

Simulation



$$R \neq R_{exp}$$

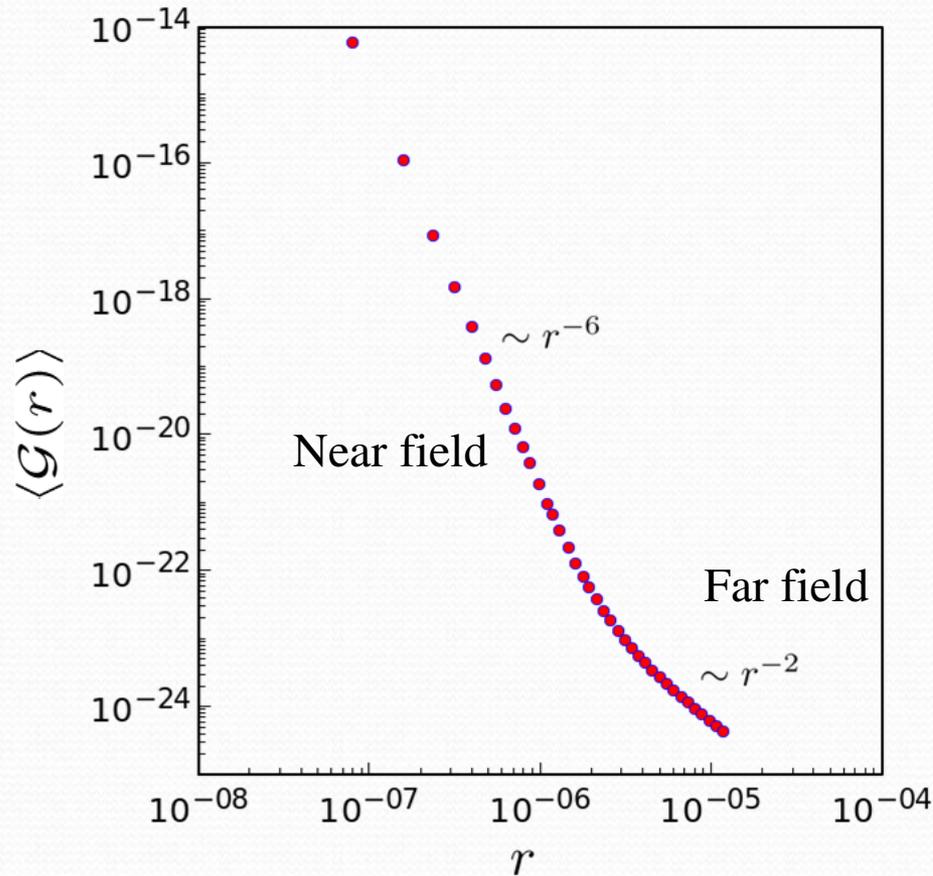
$$d \neq d_{exp}$$

$$d/R = (4\pi/3)^{1/3} \sim 1.612$$

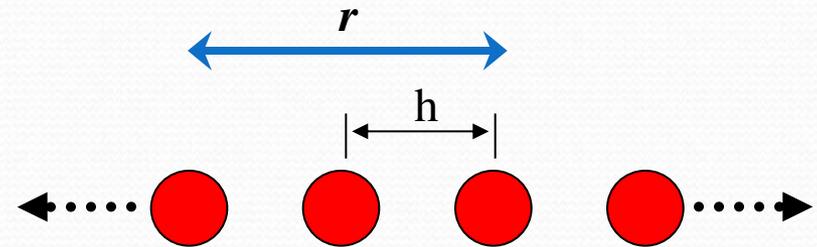
The modeled structure has the same fractal dimension, radius of gyration as the experiment one

$$R = R_{exp}(\pi/6)^{D_f/[D(D-D_f)]}$$

Mutual Conductance – 1D-Array

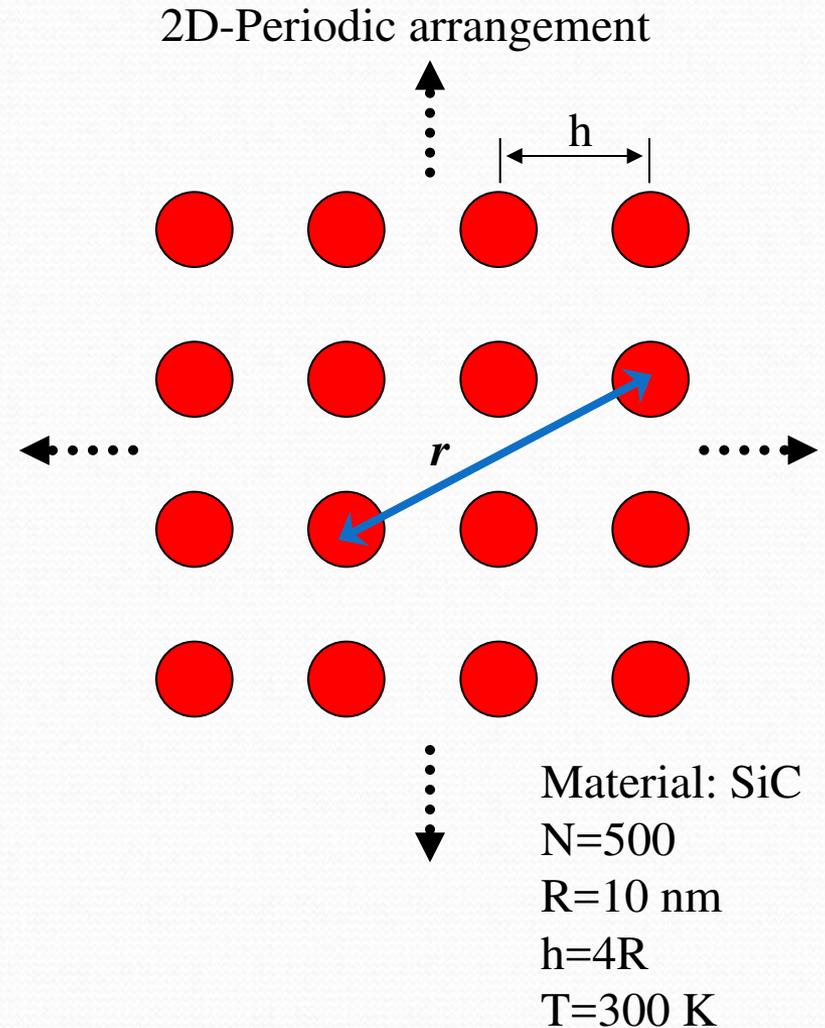
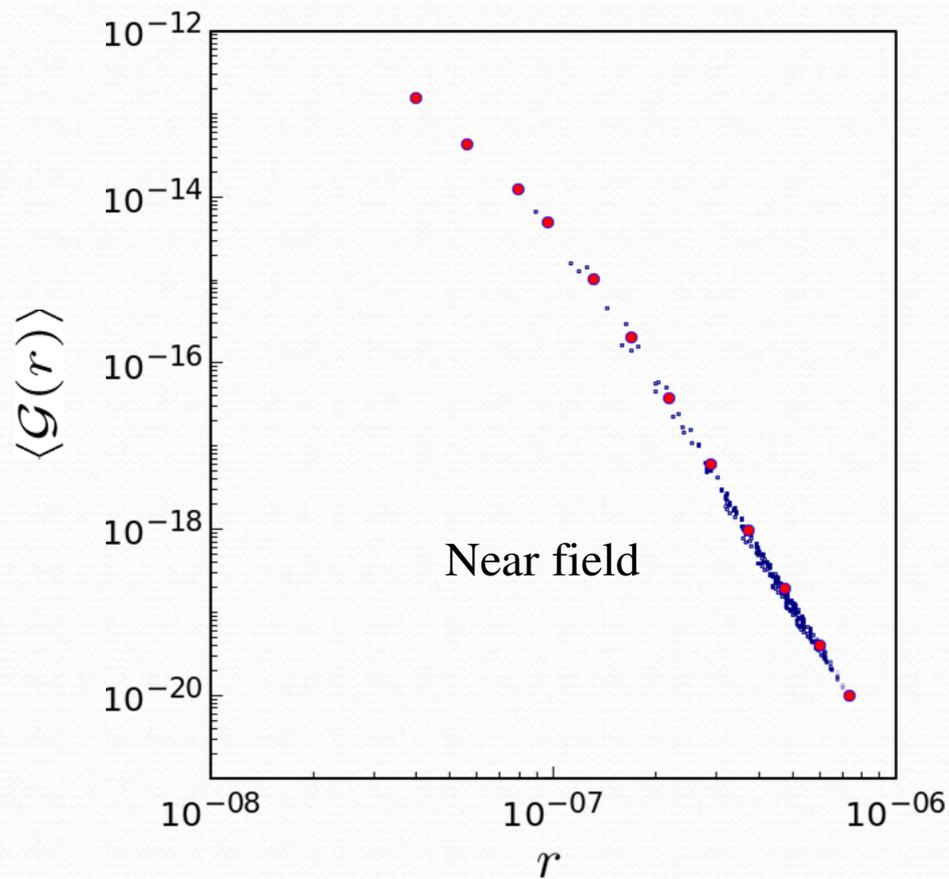


$$\mathcal{G}(r) = \mathcal{G}(|\mathbf{r}_i - \mathbf{r}_j|) = \frac{\partial \mathcal{H}_{ij}}{\partial \mathbf{T}}$$

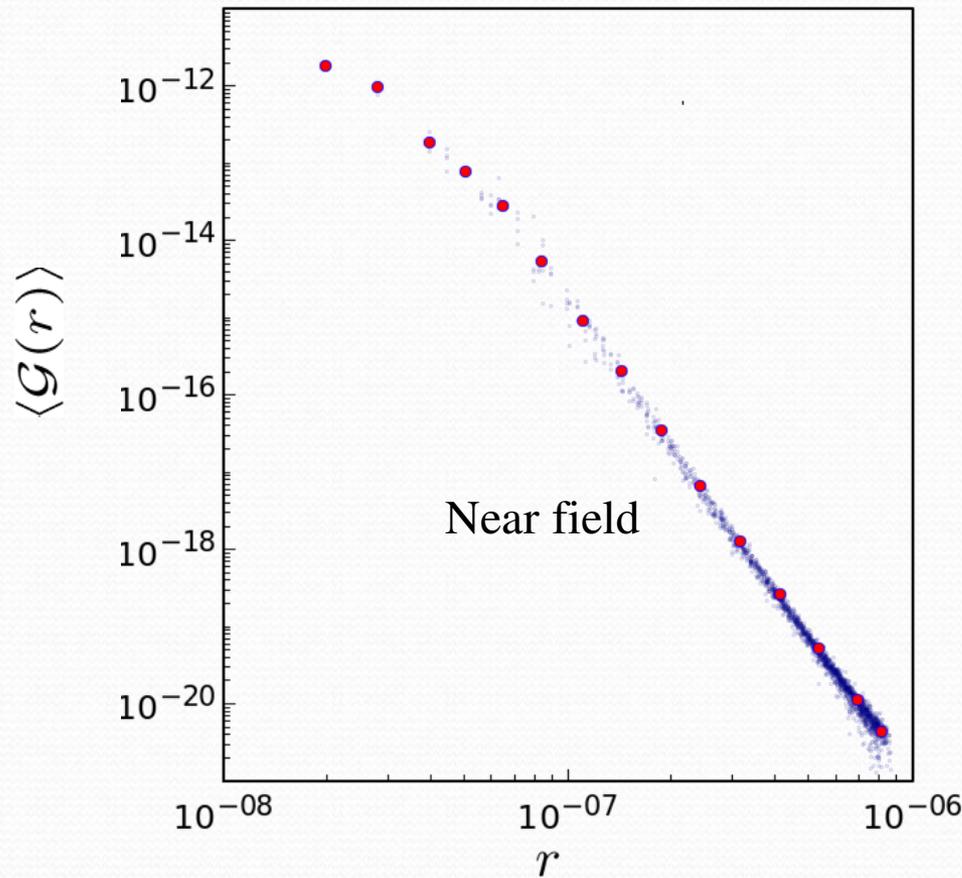


Material: SiC
N=500
R=10 nm
h=6R
T=300 K

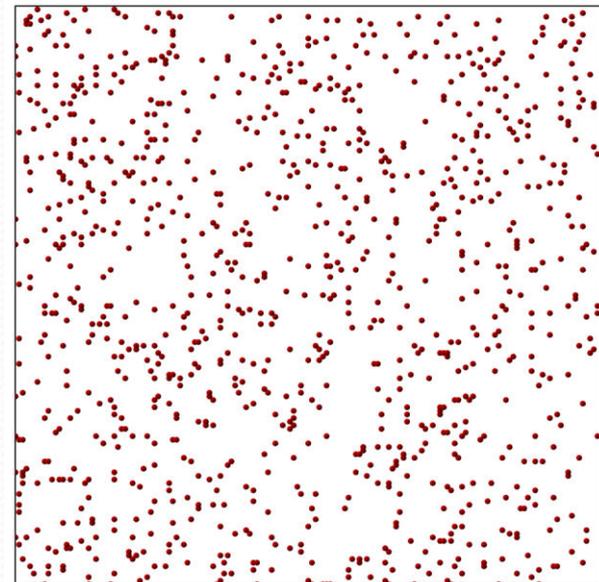
Mutual Conductance – 2D-Array



Mutual Conductance – Random distribution

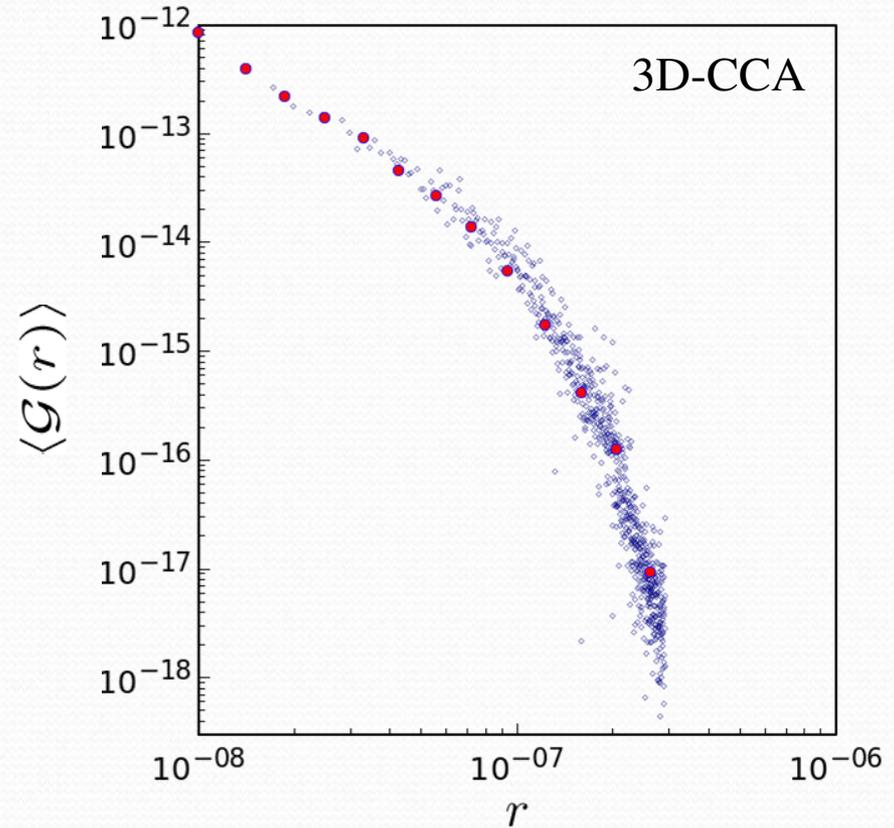
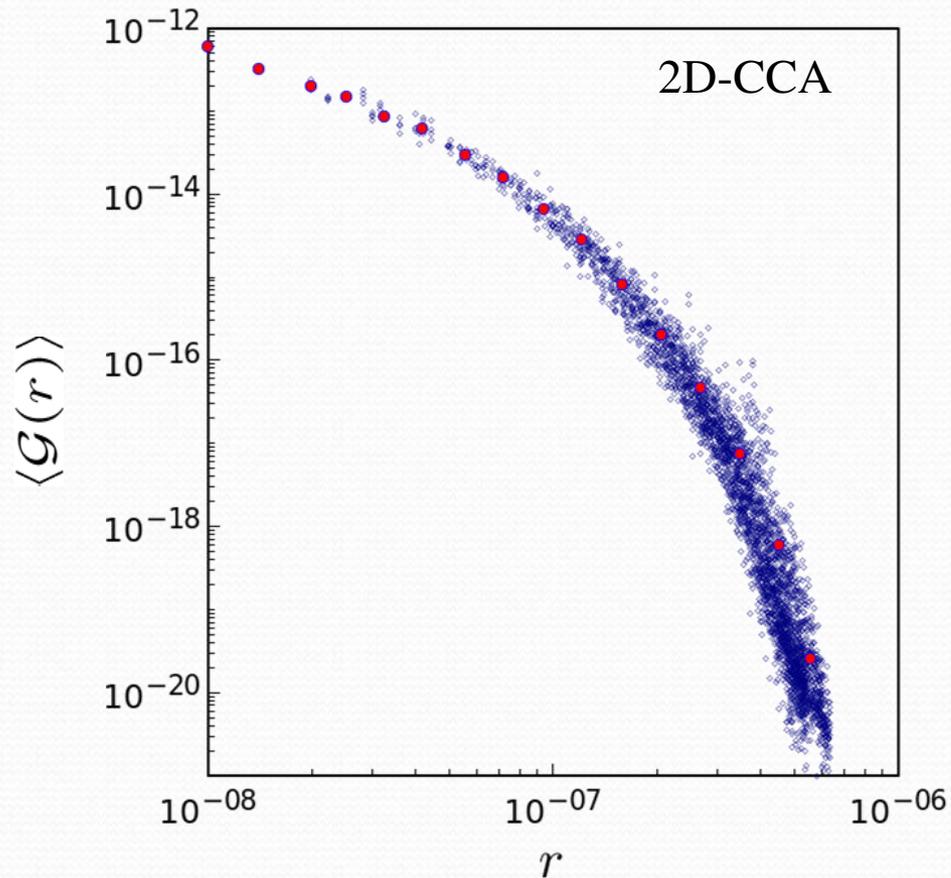


2D-Random distribution



Material: SiC $N=500$
R=10 nm Filling fraction=0.05
T=300 K Samples: 50

Mutual Conductance – Fractals

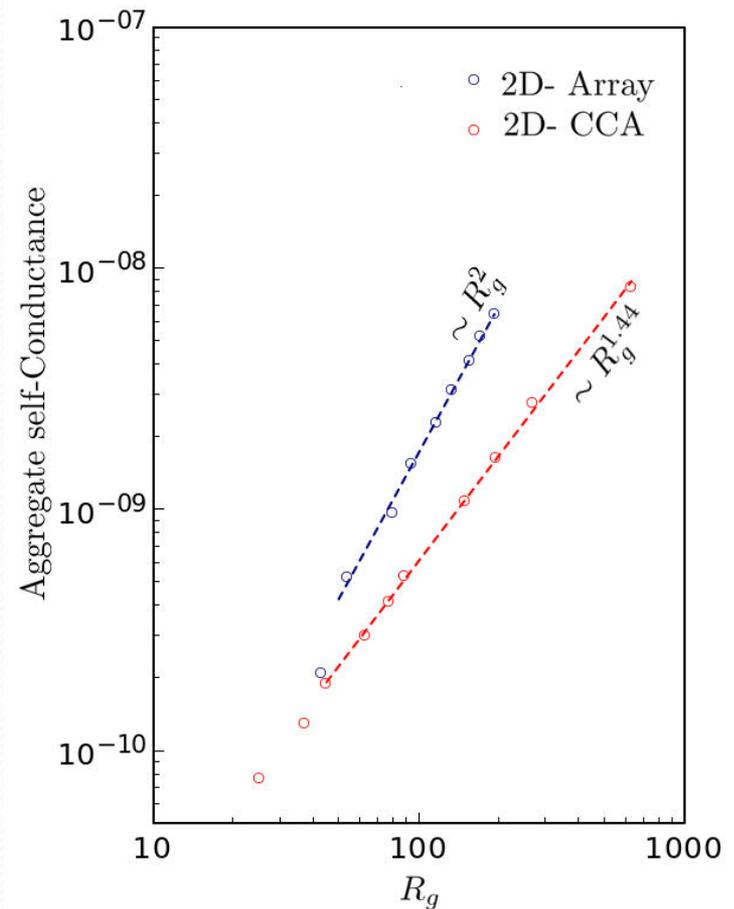
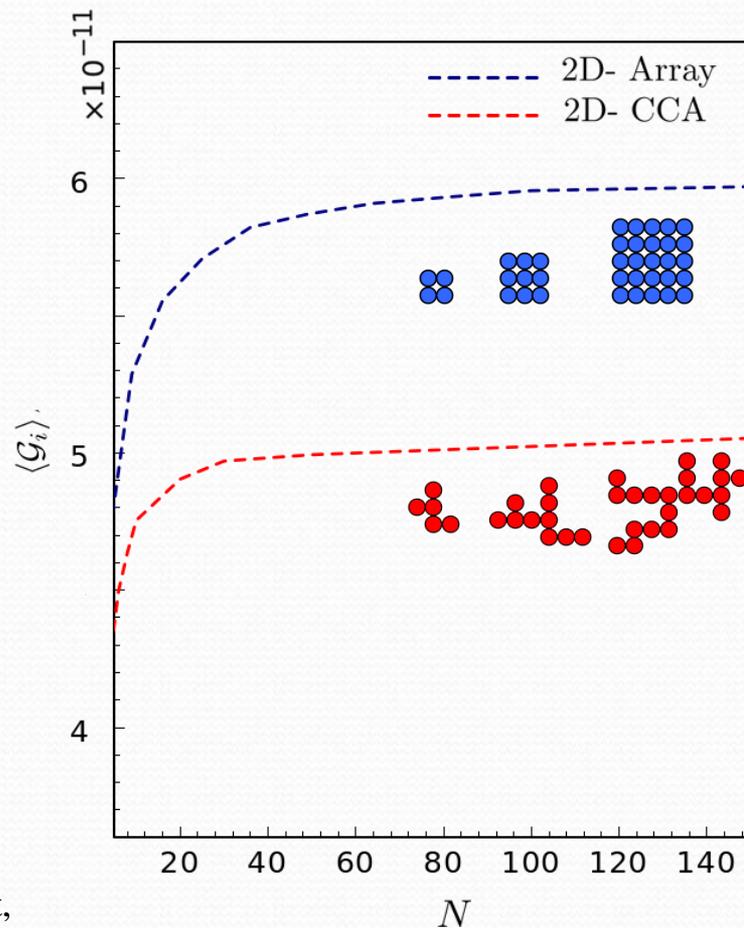


Material: SiC N=500 $R_{\text{exp}}=10$ nm T=300 K Samples: 50

Self Conductance

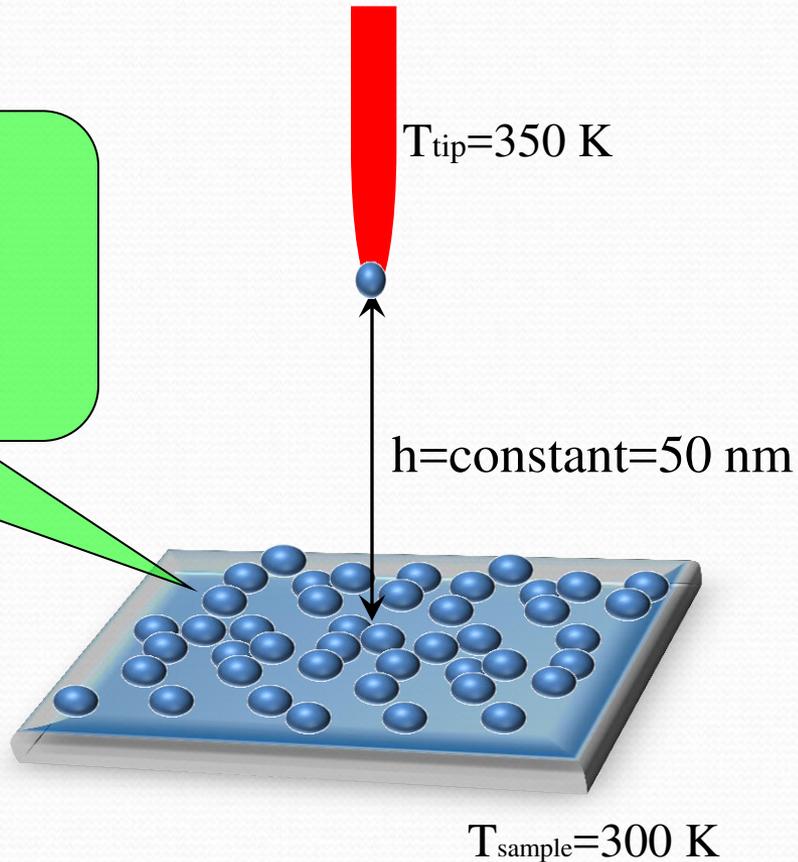
$$G_i = \frac{\partial \mathcal{F}_i}{\partial T}$$

Related to the radiative cooling of nanoparticles: Saturates as the cluster size increase



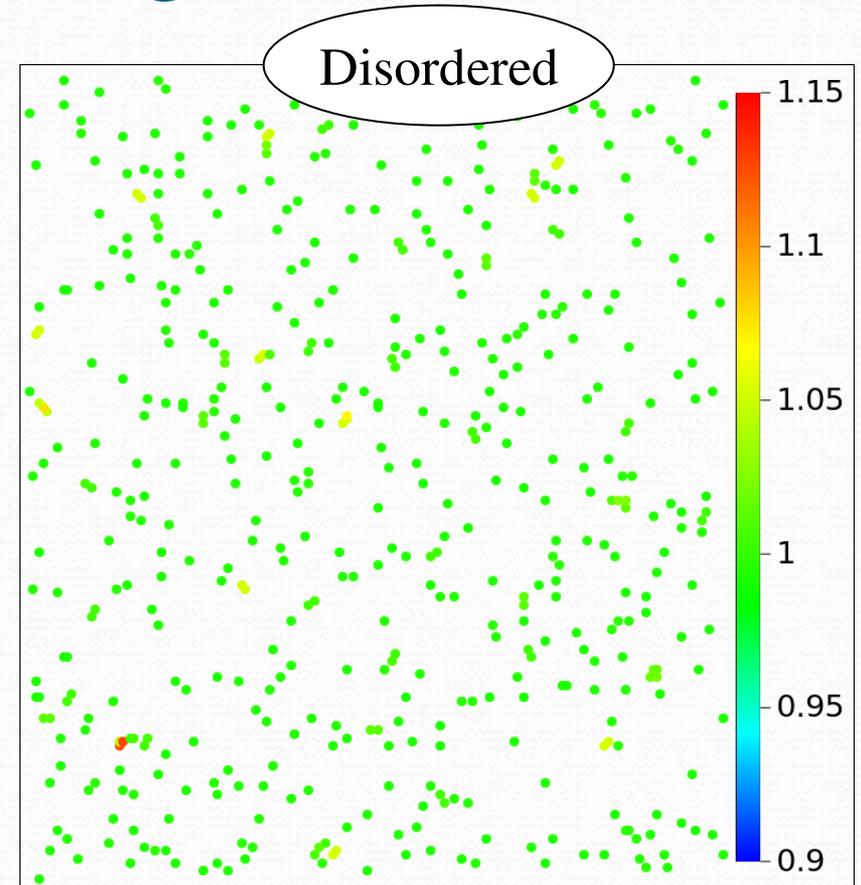
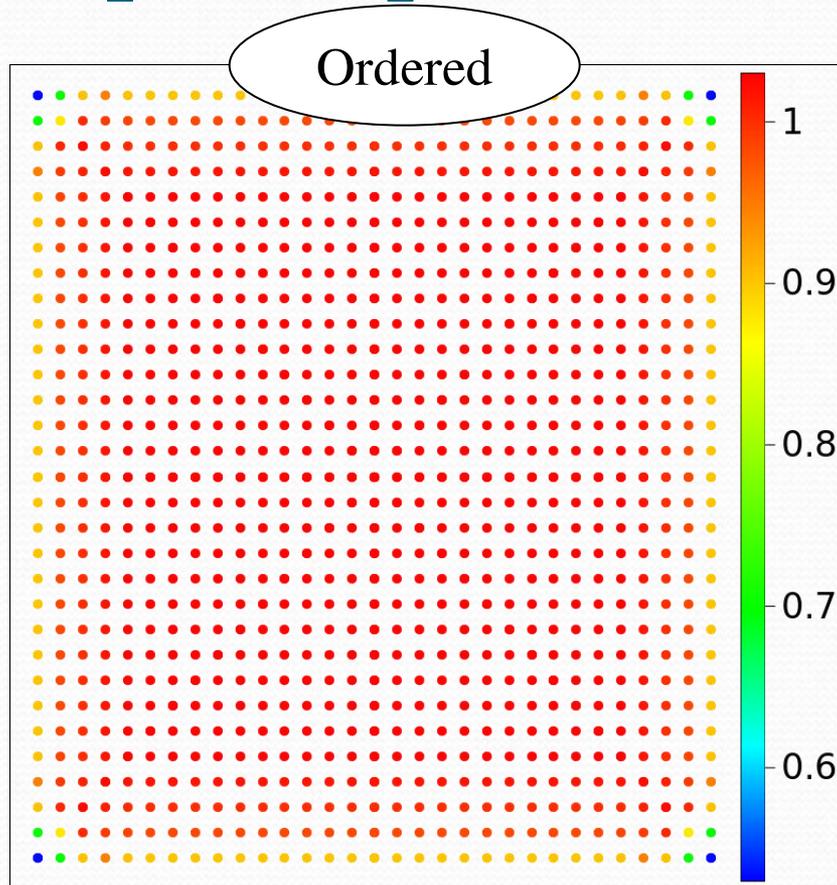
Tip-Sample Heat-Exchange

- Periodic arrangement of NPs
- Random distribution of NPs
- Fractal aggregated NPs



The tip scans the sample and the net tip-sample heat exchange is calculated

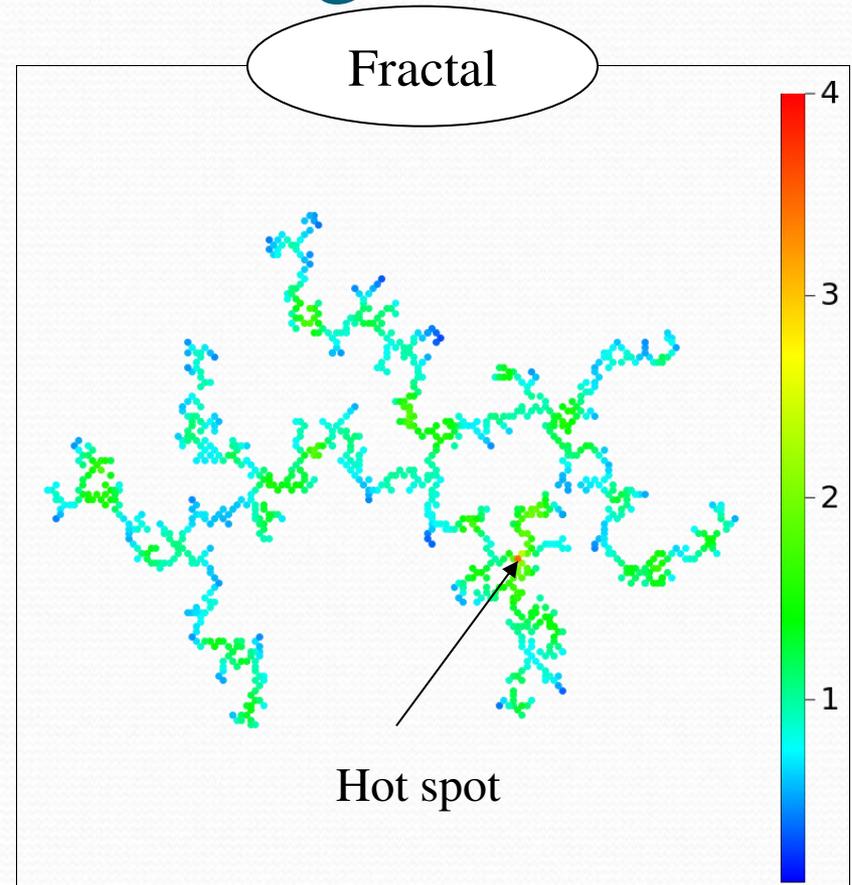
Tip-Sample Heat-Exchange (Non-fractal)



- ✓ Far a way the boundary, small fluctuation in HE compared to the average tip-sample HE
- ✓ Heat exchange is almost constant.

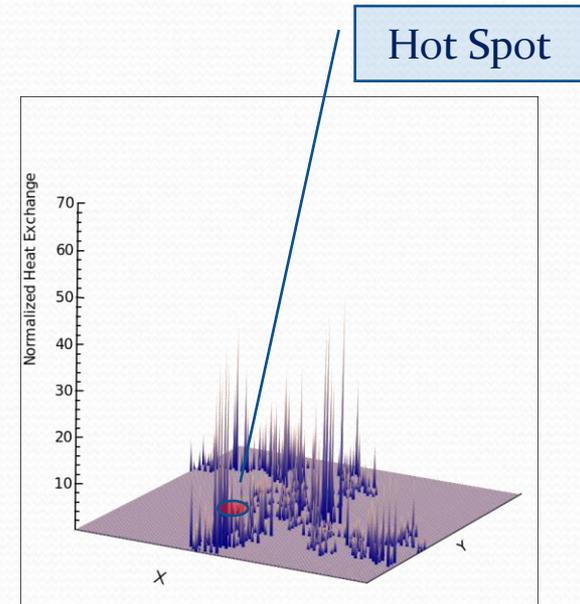
Tip-Sample Heat-Exchange (Fractal)

- ✓ Large fluctuation in heat-exchange compared to the average tip-sample heat-exchange.
- ✓ Heat exchange is localized on some places almost constant.
- ✓ The tip-sample heat-exchange in these hot spots is large.



Position of hotspot and Heat-Exchange enhancement

- Strongly depends on the geometrical structure.
- Tip-Sample Separation distance
- Nanoparticles sizes
- Nanoparticles optical properties.
- Difference between Tip and Sample optical properties



Thanks !