Title: Modelling Materials Microstructure Across Scales using Phase Field Methods

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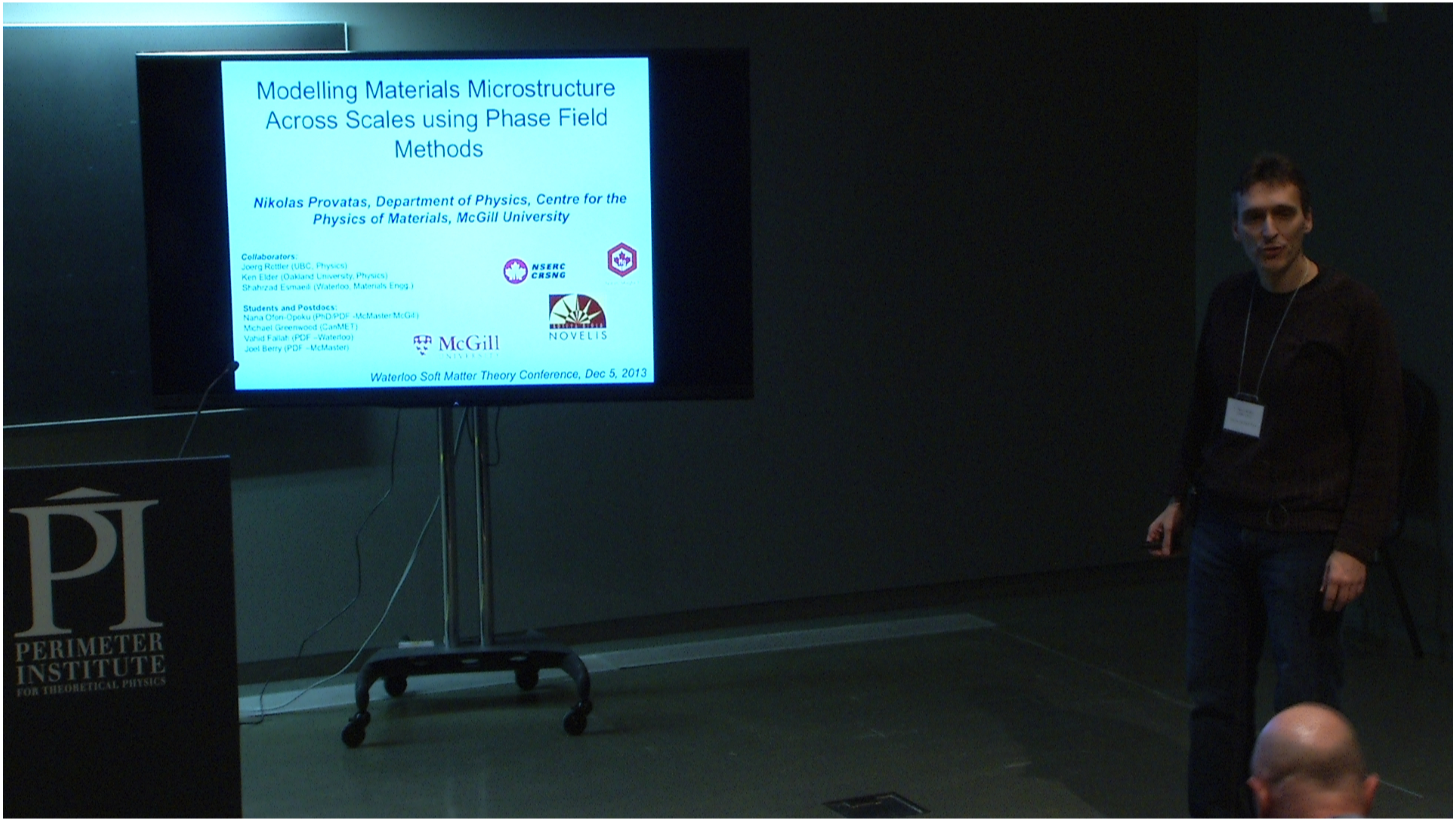
Abstract: Phase field crystal models and their recent extension will be summarized. Their application to non-equilibrium kinetics and phase transformations in materials will be reviewed. In particular, we review new results from applications of this modeling paradigm to solute trapping during rapid solidification of alloys, defect-mediated solid-state precipitation, and magneto-crystalline interactions. We close with a discussion of new complex amplitude representations of PFC models and how these can be used for multi-scale simulations using adaptive mesh refinement methods.



Modelling Materials Microstructure Across Scales using Phase Field Methods
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Collaborators:
Joerg Rottler (UBC, Physics)
Ken Elder (Oakland University, Physics)
Shahrzad Esmaeili (Waterloo, Materials Engg.)
Students and Postdocs:
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Michael Greenwood (CanMET)
Vahid Fallah (PDF -Waterloo)
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NSERC
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NOVELIS
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Waterloo Soft Matter Theory Conference, Dec 5, 2013
PERIMETER INSTITUTE FOR THEORETICAL PHYSICS

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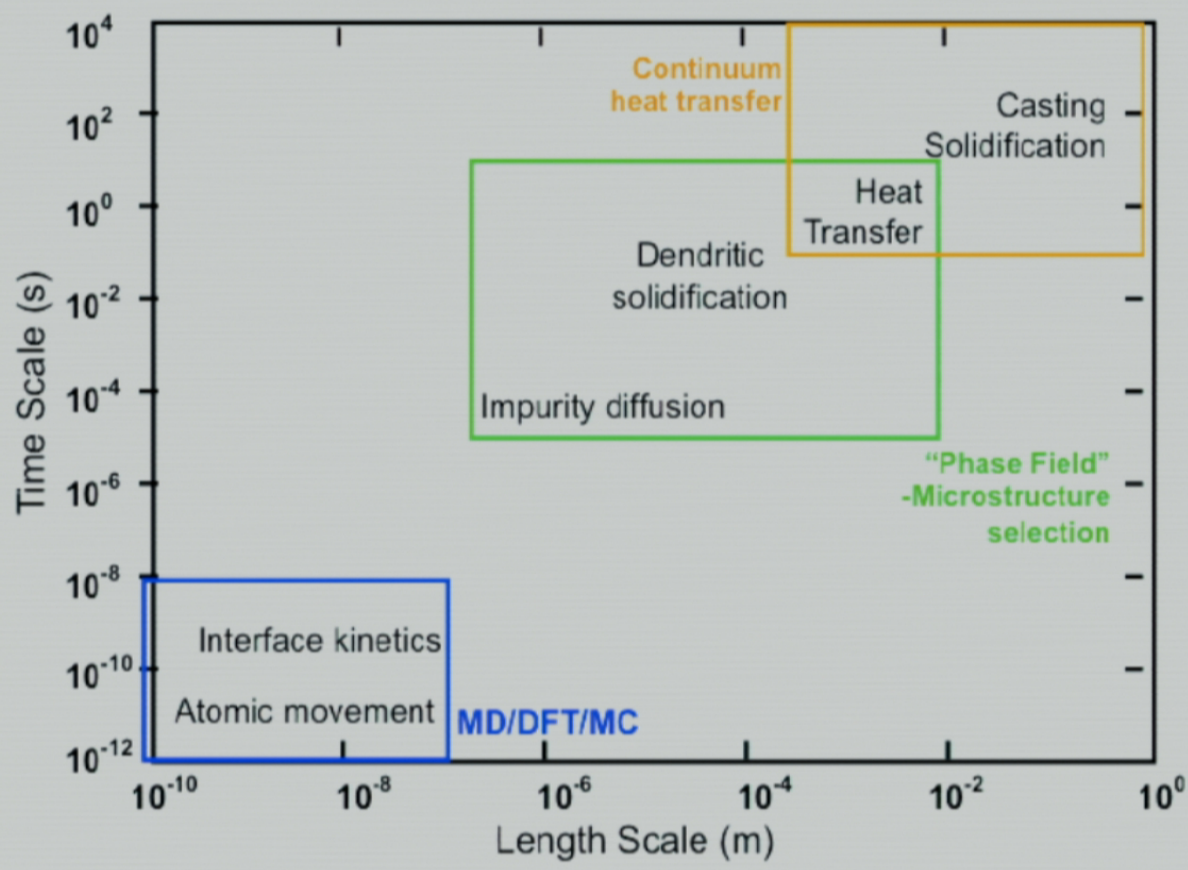
McGill UNIVERSITY

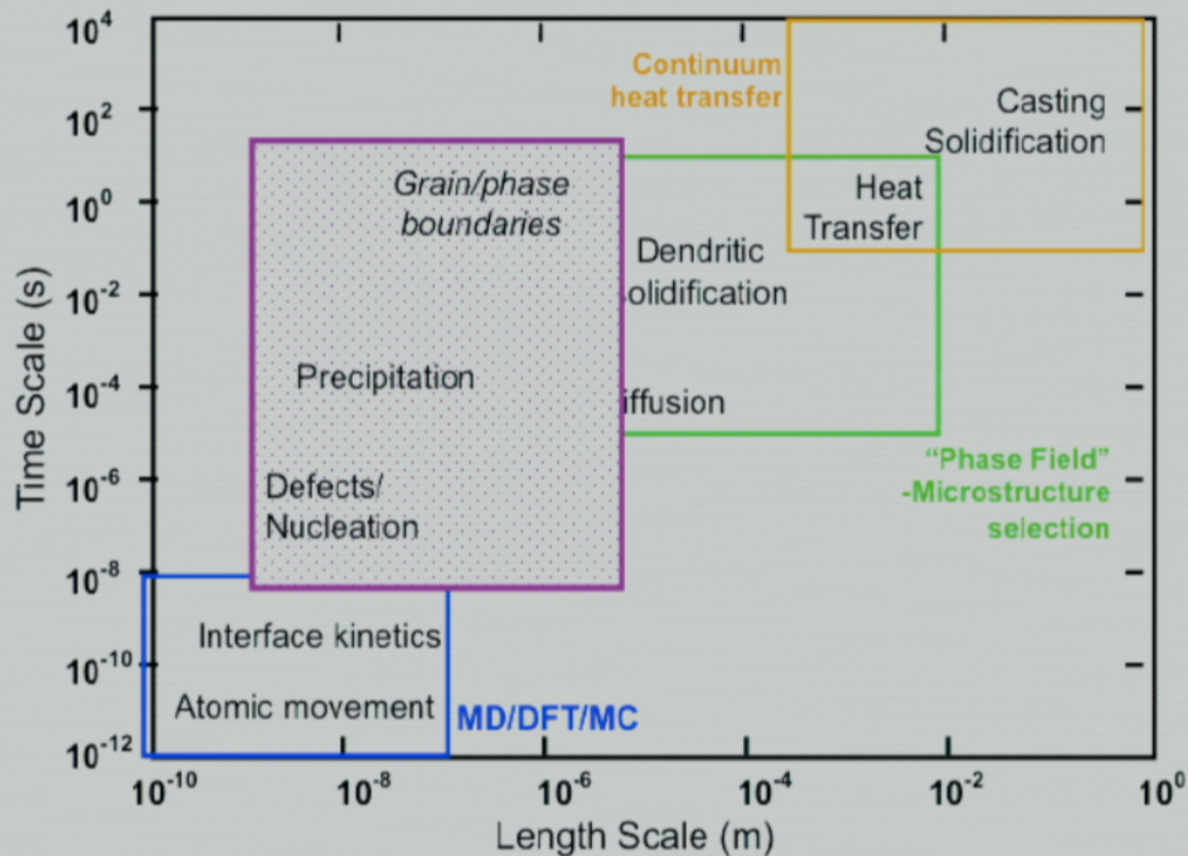
ADITYA BIRLA NOVELIS

Waterloo Soft Matter Theory Conference, Dec 5, 2013

Modeling Atomistic Effects on Diffusional Time Scales

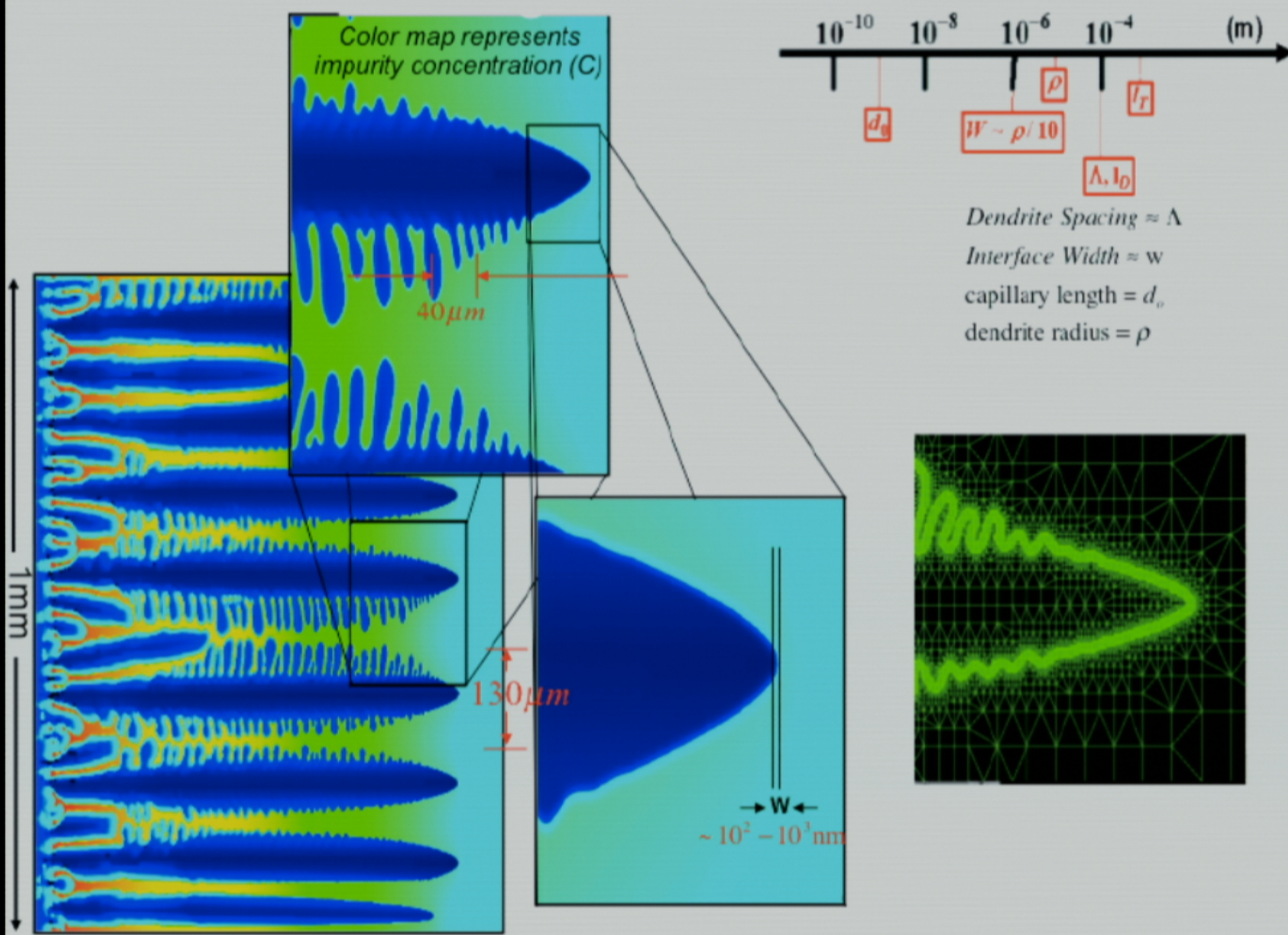


Modeling Atomistic Effects on Diffusional Time Scales



g Atomistic Effects on Diffusional Time Scales
Casting Solidification
Grain/phase boundaries
Heat Transfer
Dendritic olidification
Precipitation
ffusion
Defects/ Nucleation
Interface kinetics
Atomic movement
MD/DFT/MC
10^-10
10^-8
10^-6
10^-4
10^-2
10^0
Length Scale (m)

Phase Field Models of Solidification



Periodic Order Parameters

$$n = \frac{\rho - \rho_o}{\rho_o}$$

$$F = \frac{\mathbf{F}}{k_B T} = \frac{1}{k_B T}(F_{id} + F_{Ex})$$

F_{Ex} → Interacting Energy

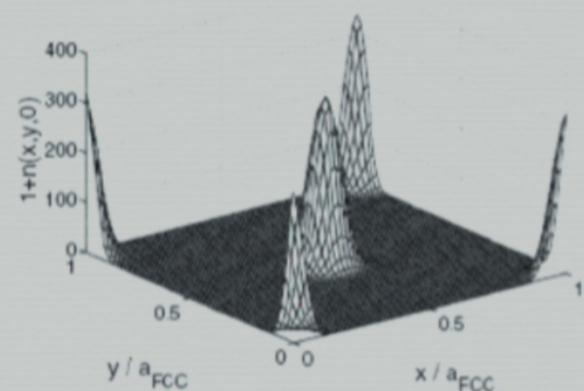
F_{id} → Non Interacting Energy

Ramakrishnan, PRB 1979

$$F_{\rm id} = \int d\vec{r} \left(\rho \ln \left(\frac{\rho}{\rho_o} \right) - \delta\rho \right) \rightarrow \int d\vec{r} \left(\frac{n^2}{2} - \frac{n^3}{2} + \frac{n^4}{12} + \cdots \right)$$

$$F_{ex} = -\frac{1}{2} \int d\vec{r}_1 \int d\vec{r}_2 \left[\Delta\rho(\vec{r}_1) C_2^{HS}(r_1, r_1, \bar{\rho}) \Delta\rho(\vec{r}_2) \right] + \ldots.$$

FCC (100) Plane



A. Jaatinen PRE 2009

Multi-Component Systems

Composition: $c_i = \dfrac{\rho_i}{\sum_{m=1}^{N} \rho_m}$

Dimensionless density: $n = \dfrac{\sum_{i=1}^{N} \rho_i}{\sum_{i=1}^{N} \rho_i^o} - 1$

Binary: **M. Greenwood, N. Ofori-Opoku, J. Rottler and N. Provatas, Acta Mater. (2011)**
N-Component: **Nana Ofori-Opoku, et al, Phys. Rev. B vol. 87 (2013)**

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$$\frac{\Delta F}{k_B T \rho^o} = \int \underbrace{\frac{n^2}{2} - \xi \frac{n^3}{6} + \chi \frac{n^4}{12} - \frac{n(\vec{r})}{2}\left(\int C_{eff}(|r-r'|) n(\vec{r}\,')\, d\vec{r}\,'\right)}_{\text{Crystallography \& defects}} + \omega \underbrace{\Delta F_{mix}\left(\{c_i\}\right)(n+1) + \frac{1}{2}\sum_{i,j=1}^{N} \kappa_{ij} \vec{\nabla} c_i \cdot \vec{\nabla} c_j}_{\text{Soute additions}} d\vec{r}$$

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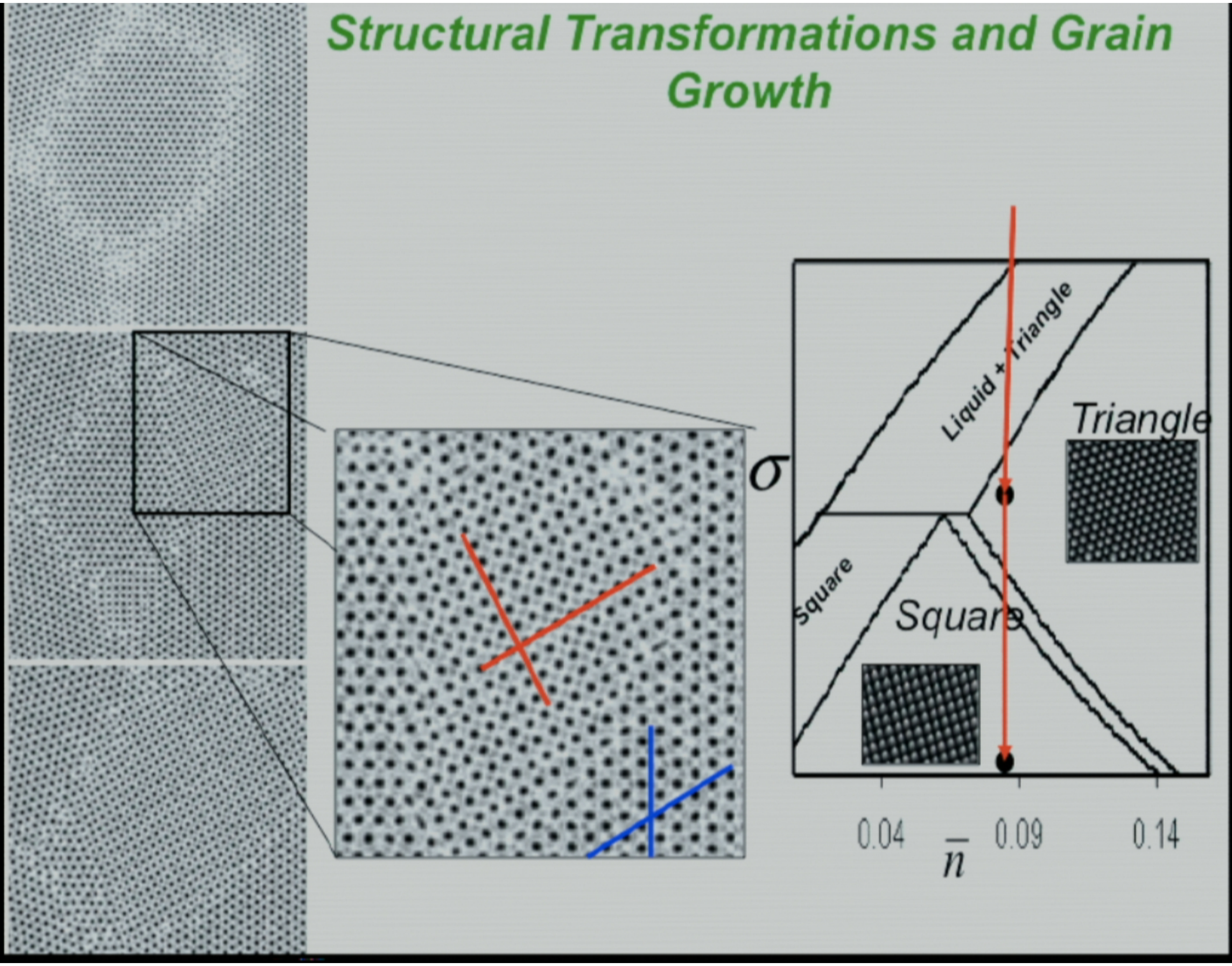
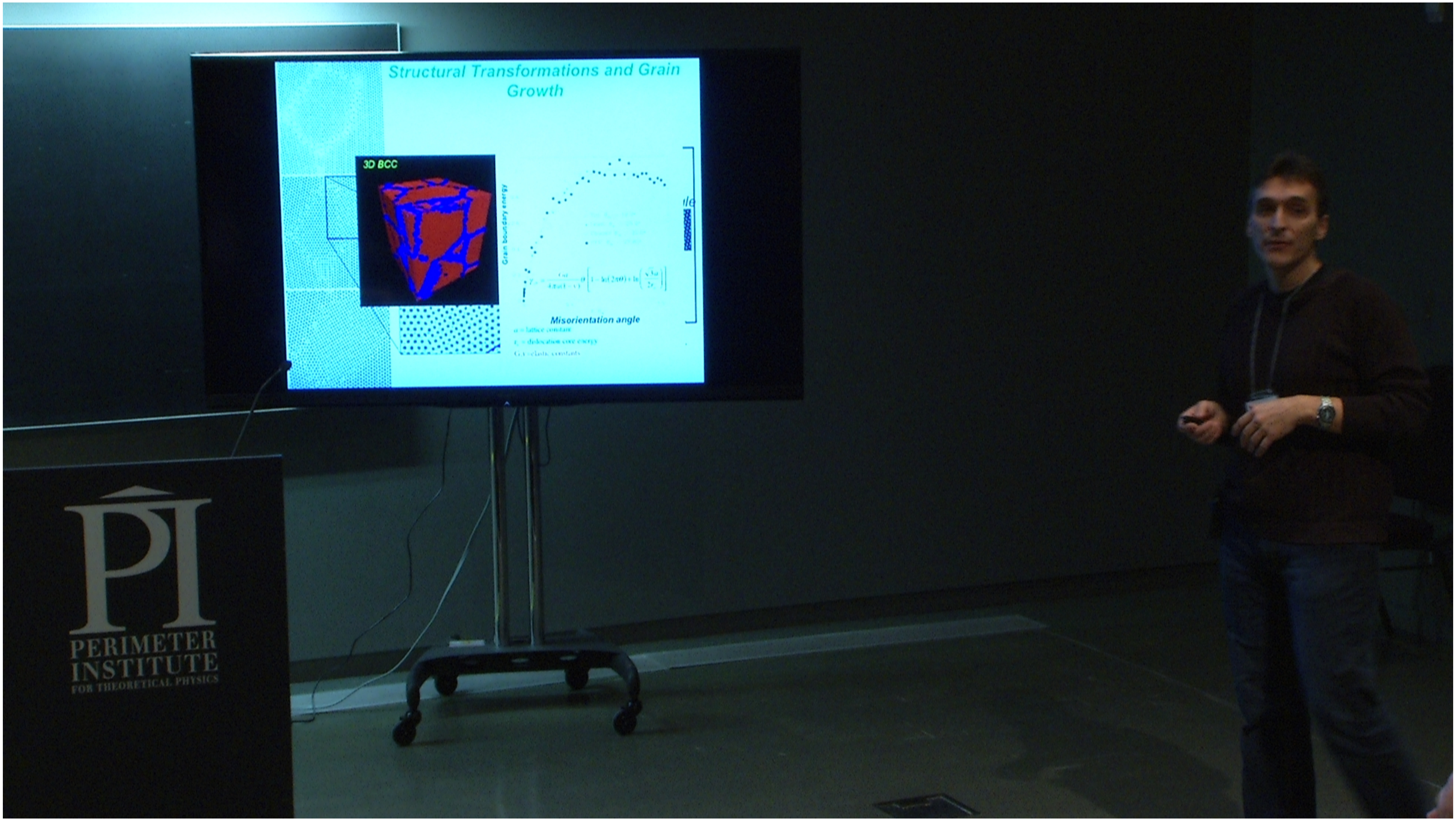
Structural Transformations and Grain Growth





Structural Transformations and Grain Growth
3D BCC
Misorientation angle
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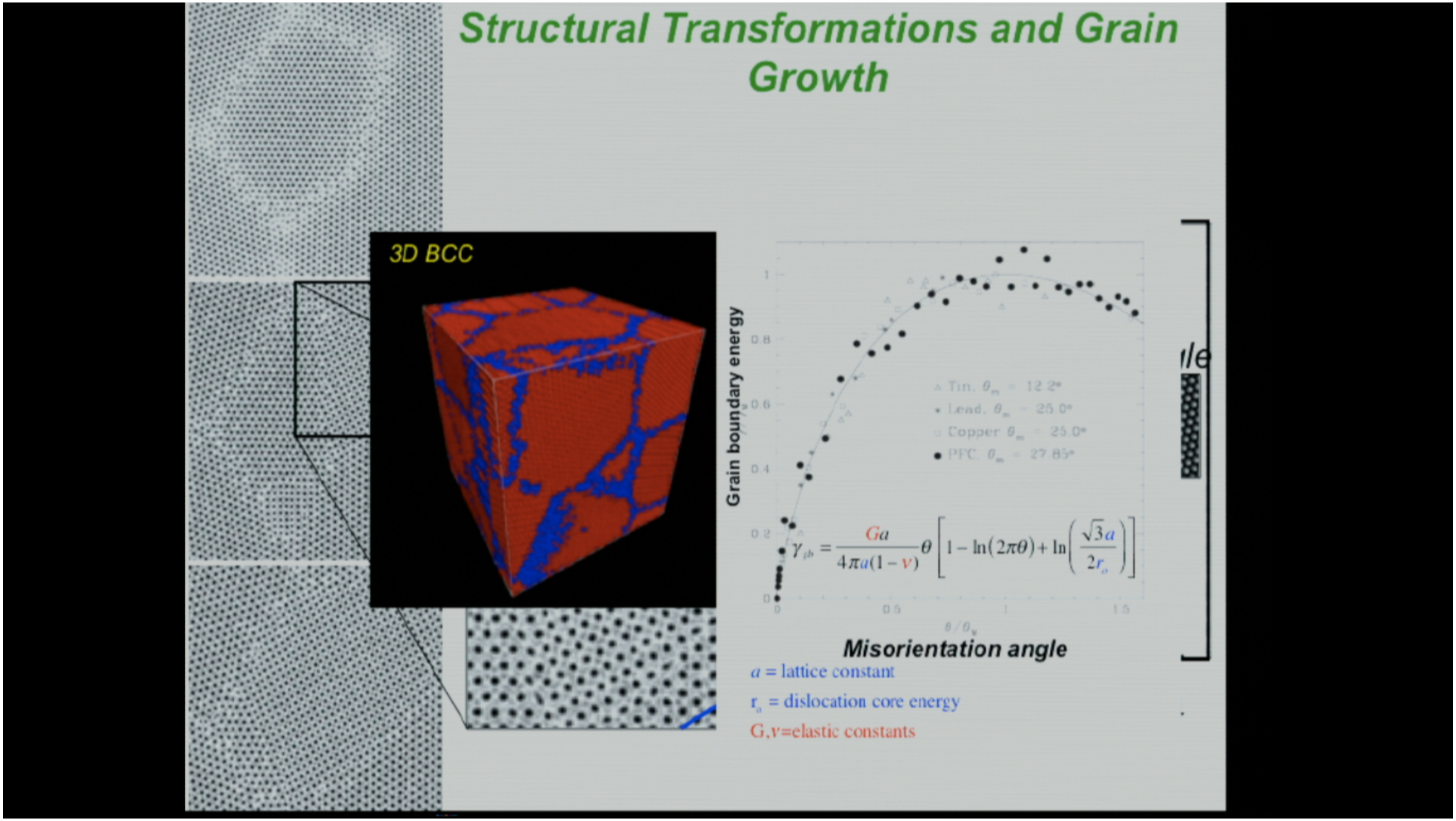
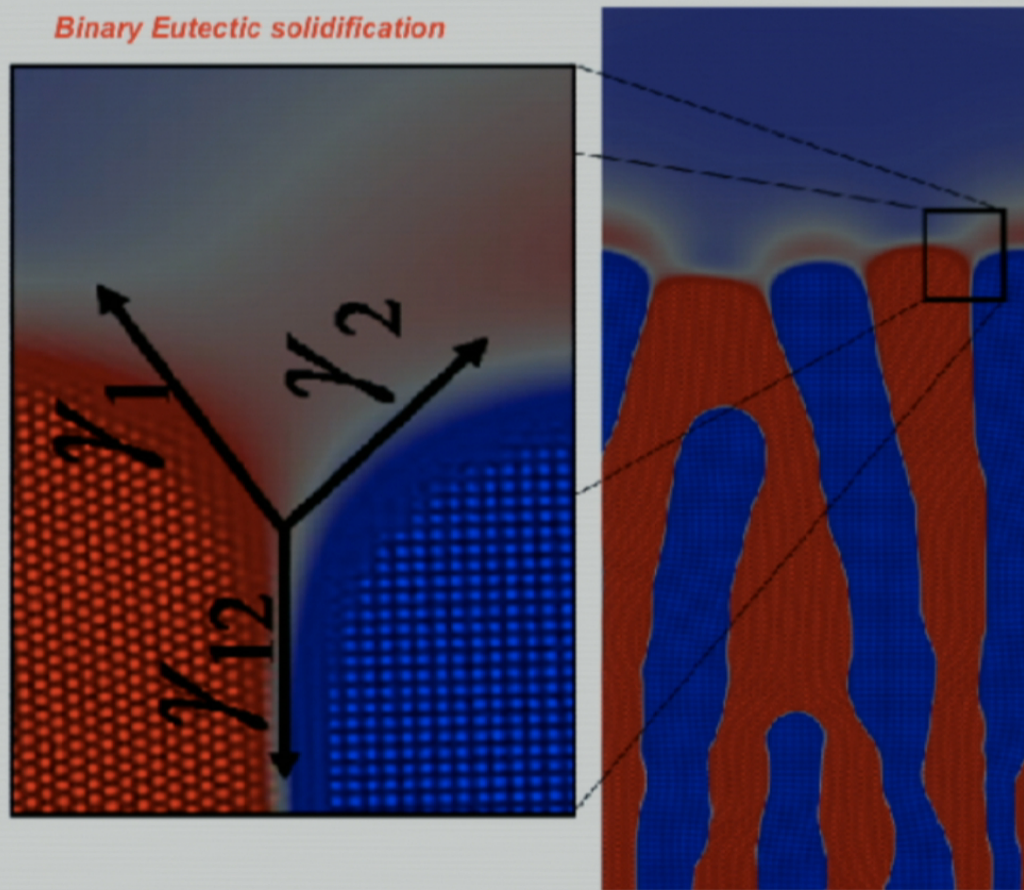
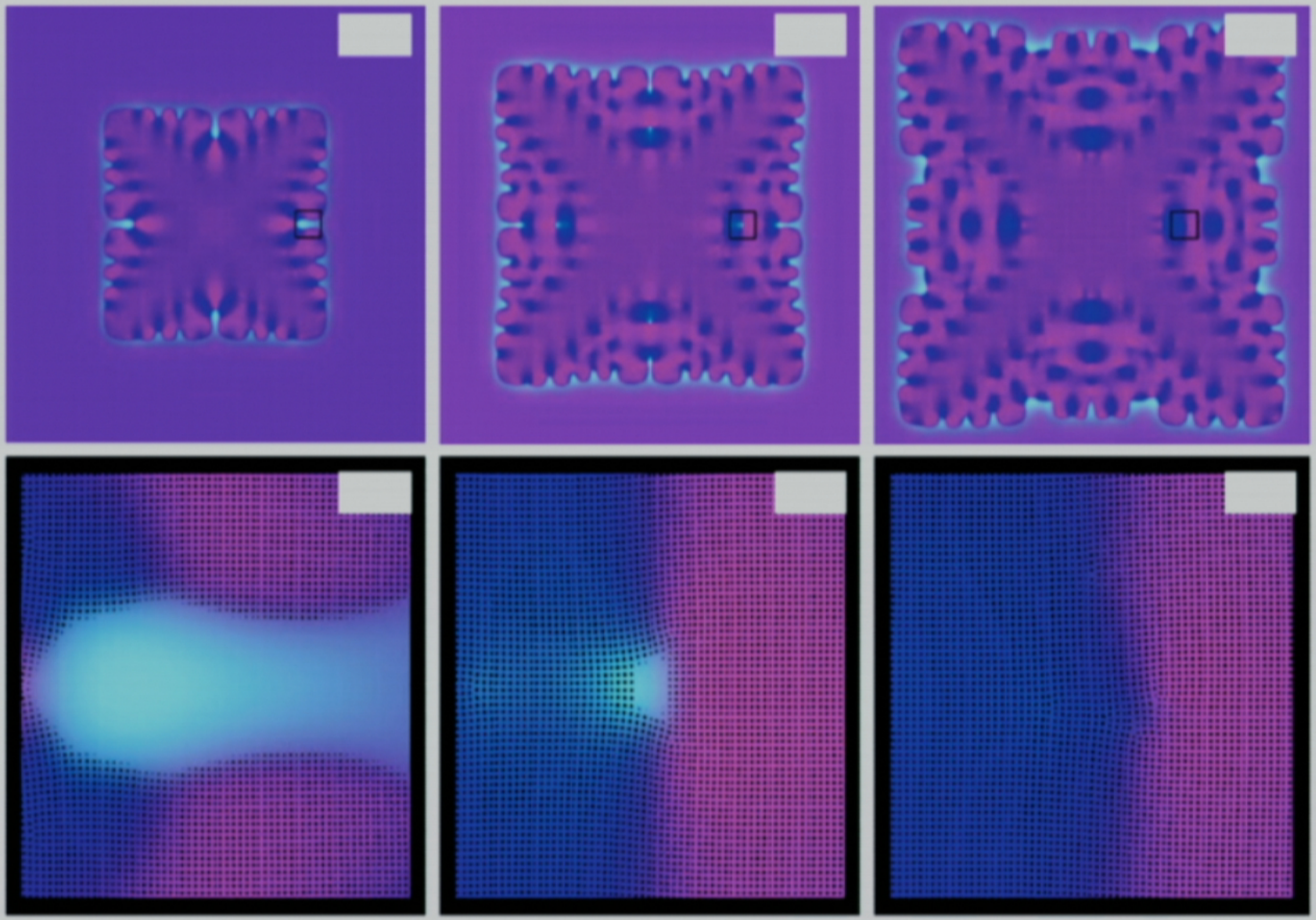

Structural Transformations and Grain Growth
3D BCC
Grain boundary energy
Misorientation angle
Tin, θ_m = 12.2°
Lead, θ_m = 25.0°
Copper θ_m = 25.0°
PFC θ_m = 27.85°
$\gamma_{gb} = \frac{Ga}{4\pi a(1-\nu)}\theta\left[1-\ln(2\pi\theta)+\ln\left(\frac{\sqrt{3}a}{2r_o}\right)\right]$
a = lattice constant
r_o = dislocation core energy
G,ν=elastic constants

Solidification of Meta-Stable Phases

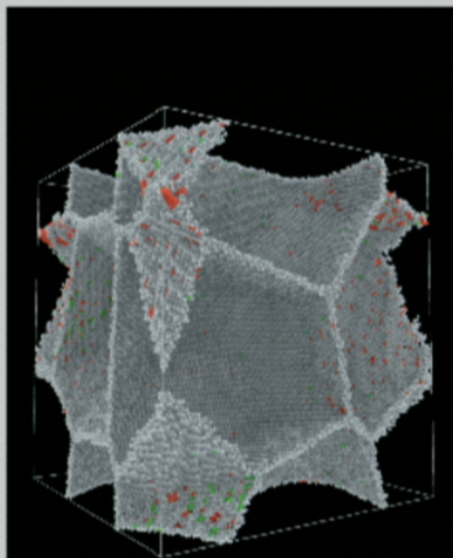


Solidification of Meta-Stable Phases

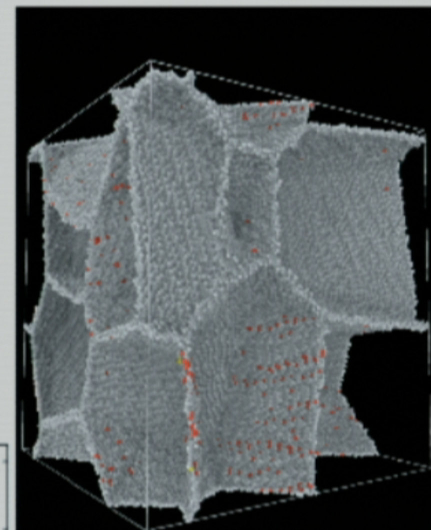


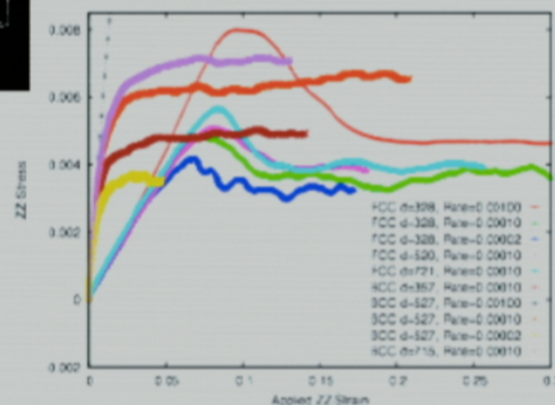
Conservative Dislocation Creation Mechanisms

FCC polycrystal deformation



BCC polycrystal deformation





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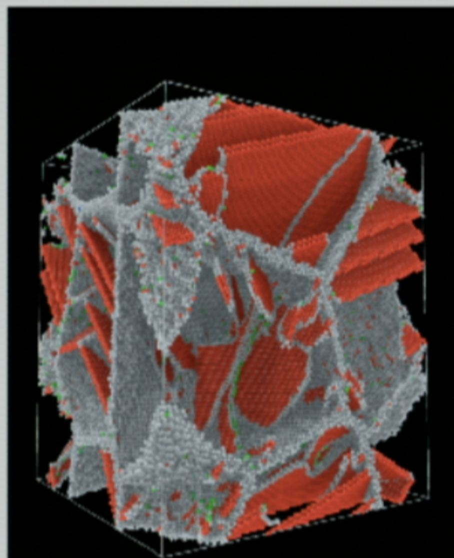

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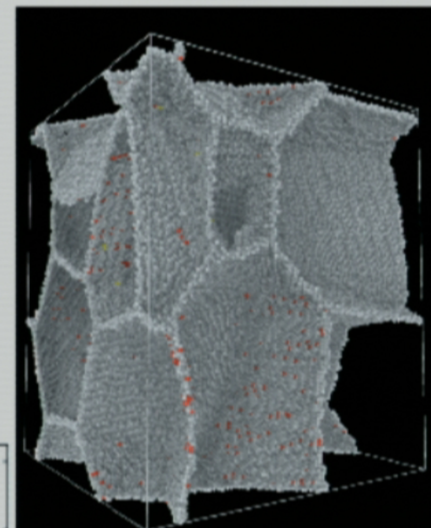

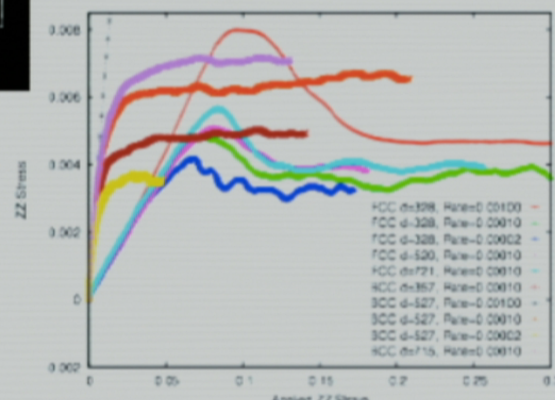

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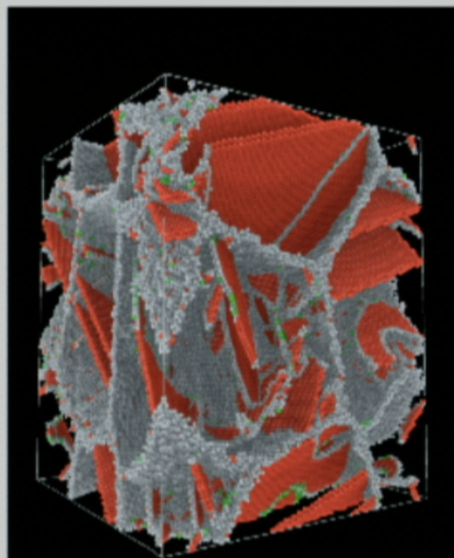
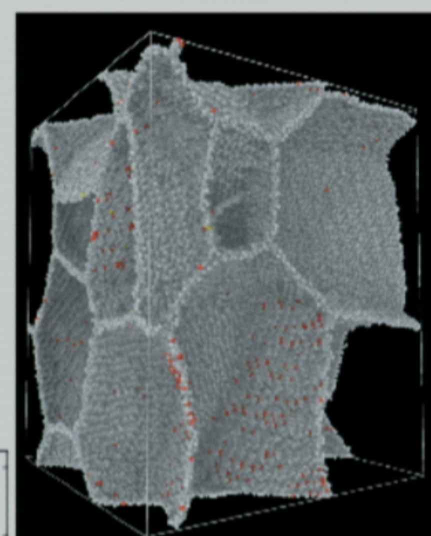
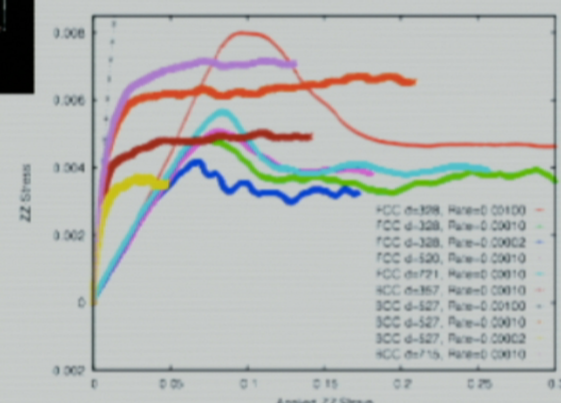


BCC polycrystal deformation





Conservative Dislocation Creation Mechanisms

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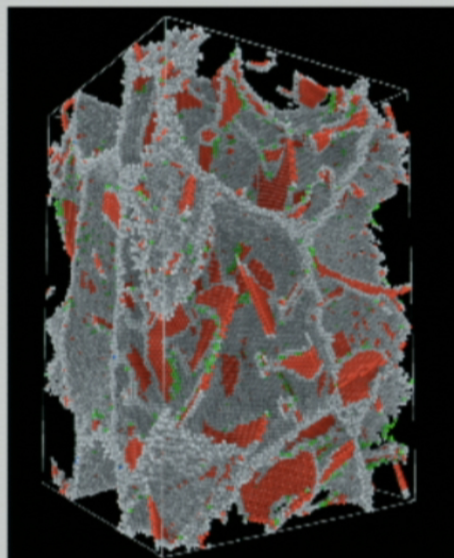

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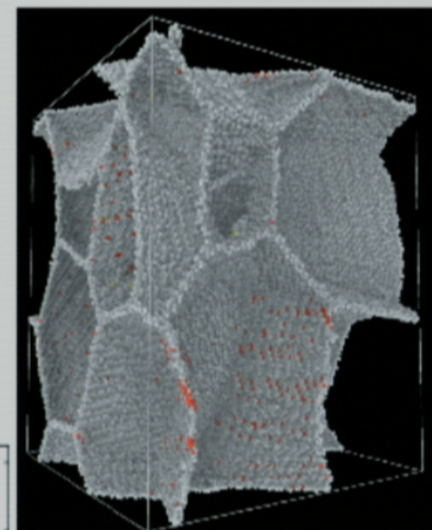
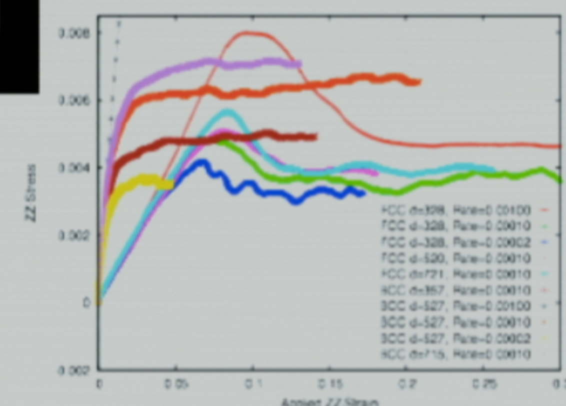
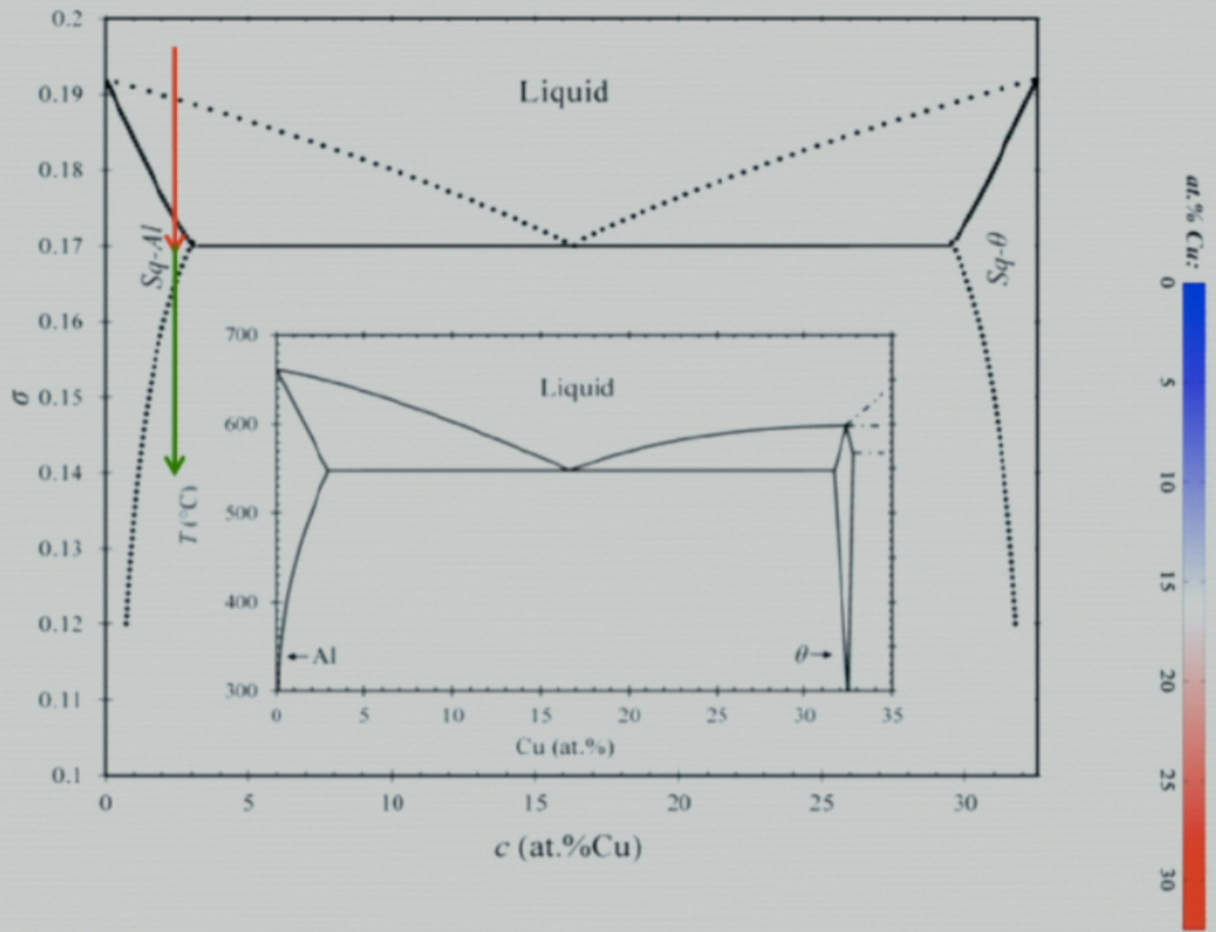




Role of Dislocations on Precipitation



[Vahid Fallah, et. Al Phys. Rev B, 86, 134112 (2012); Acta. Mat., 61, 6372 (2013)]

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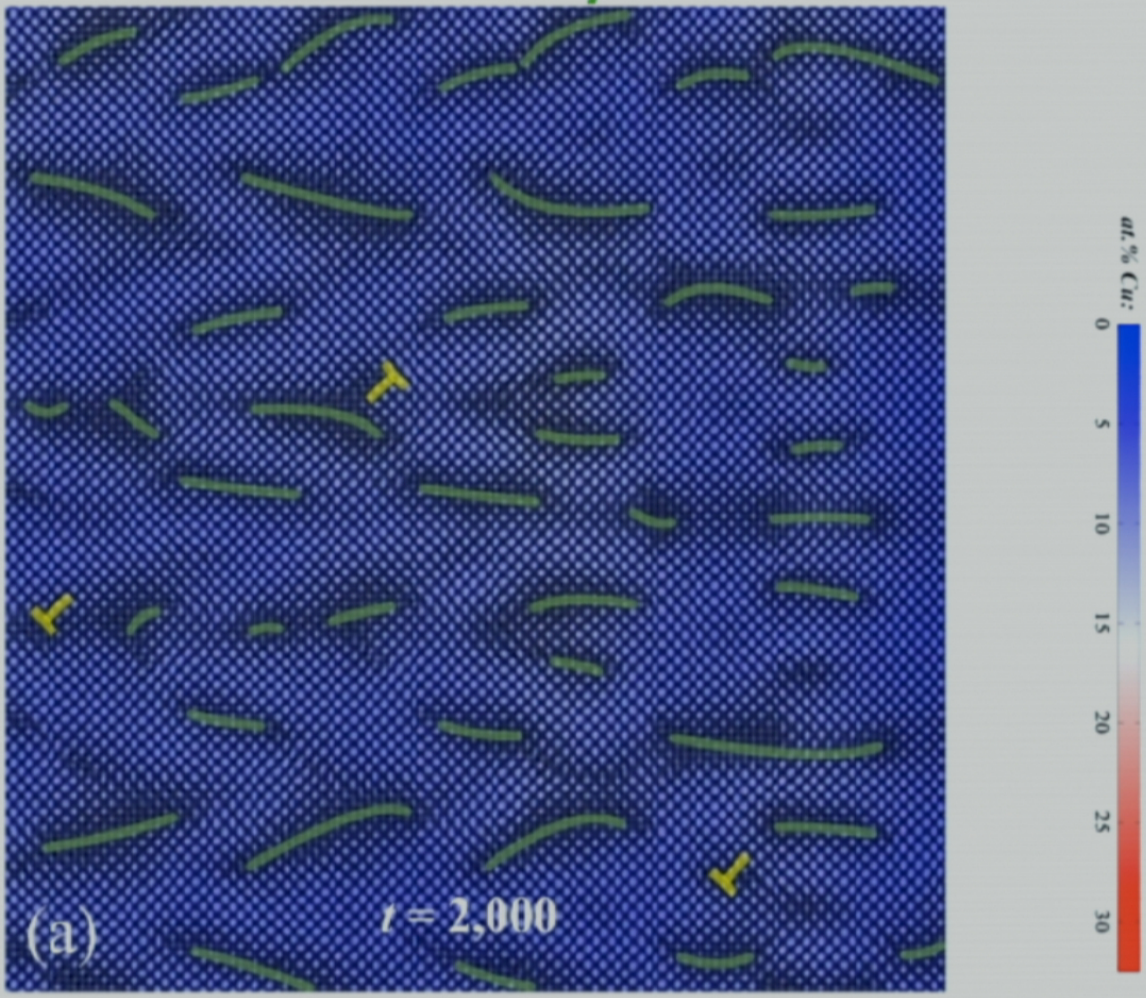

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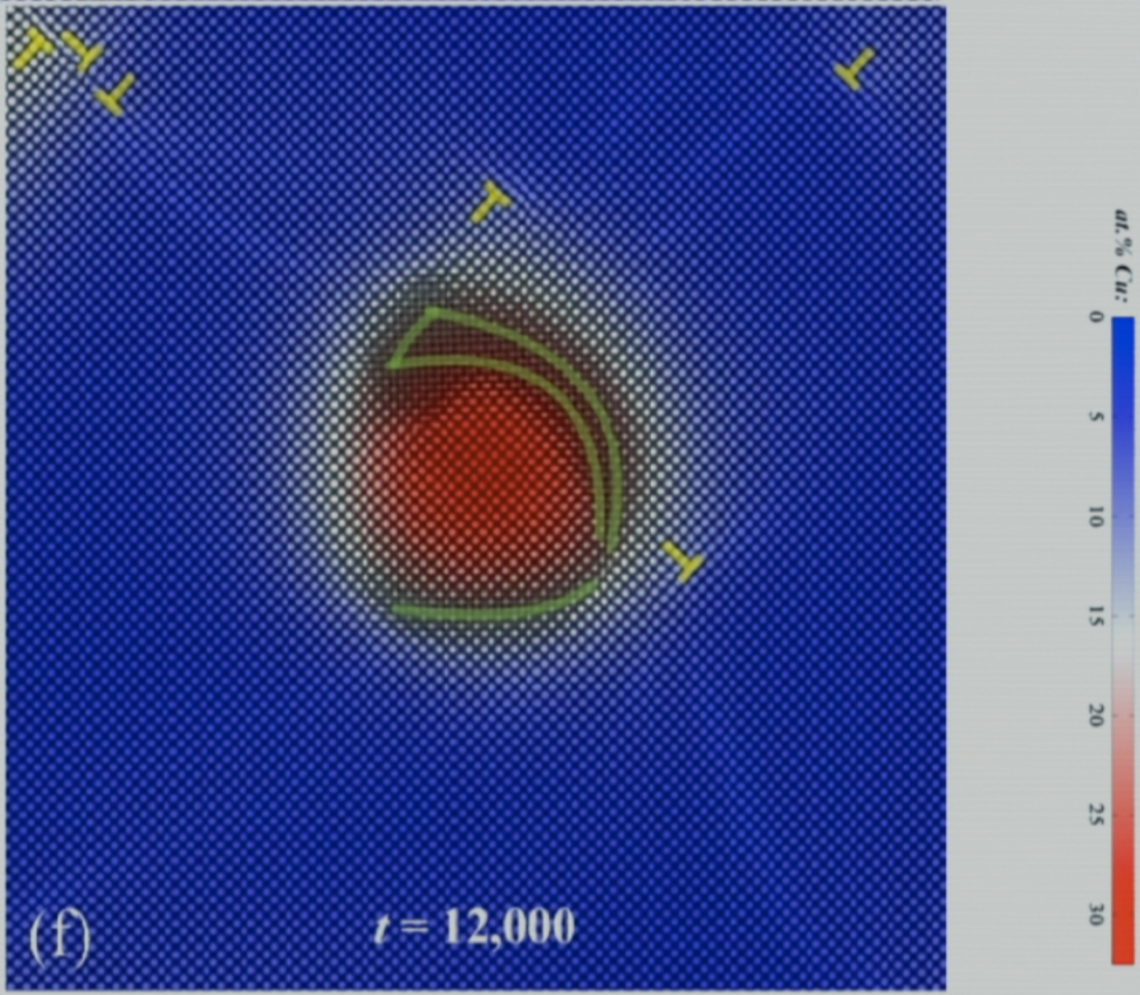

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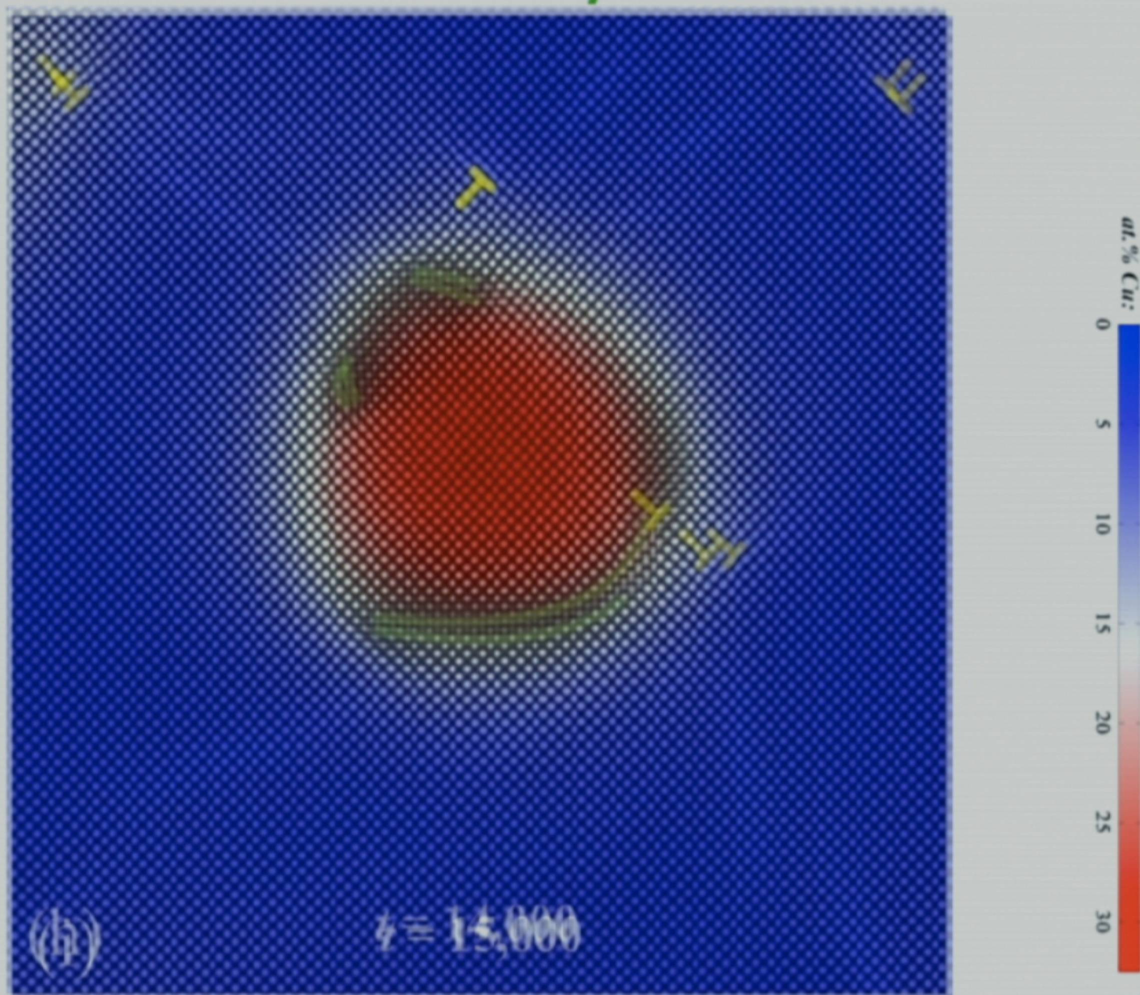

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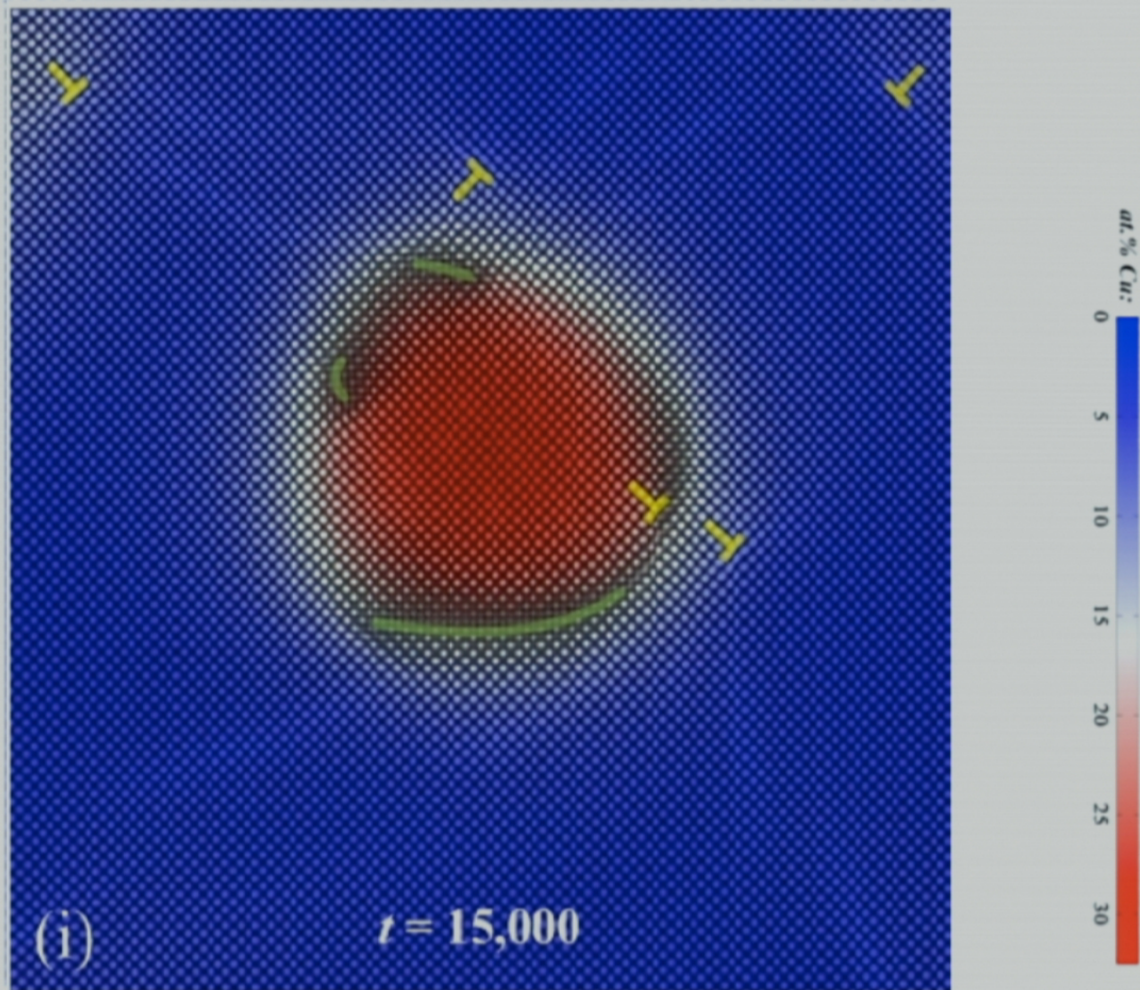

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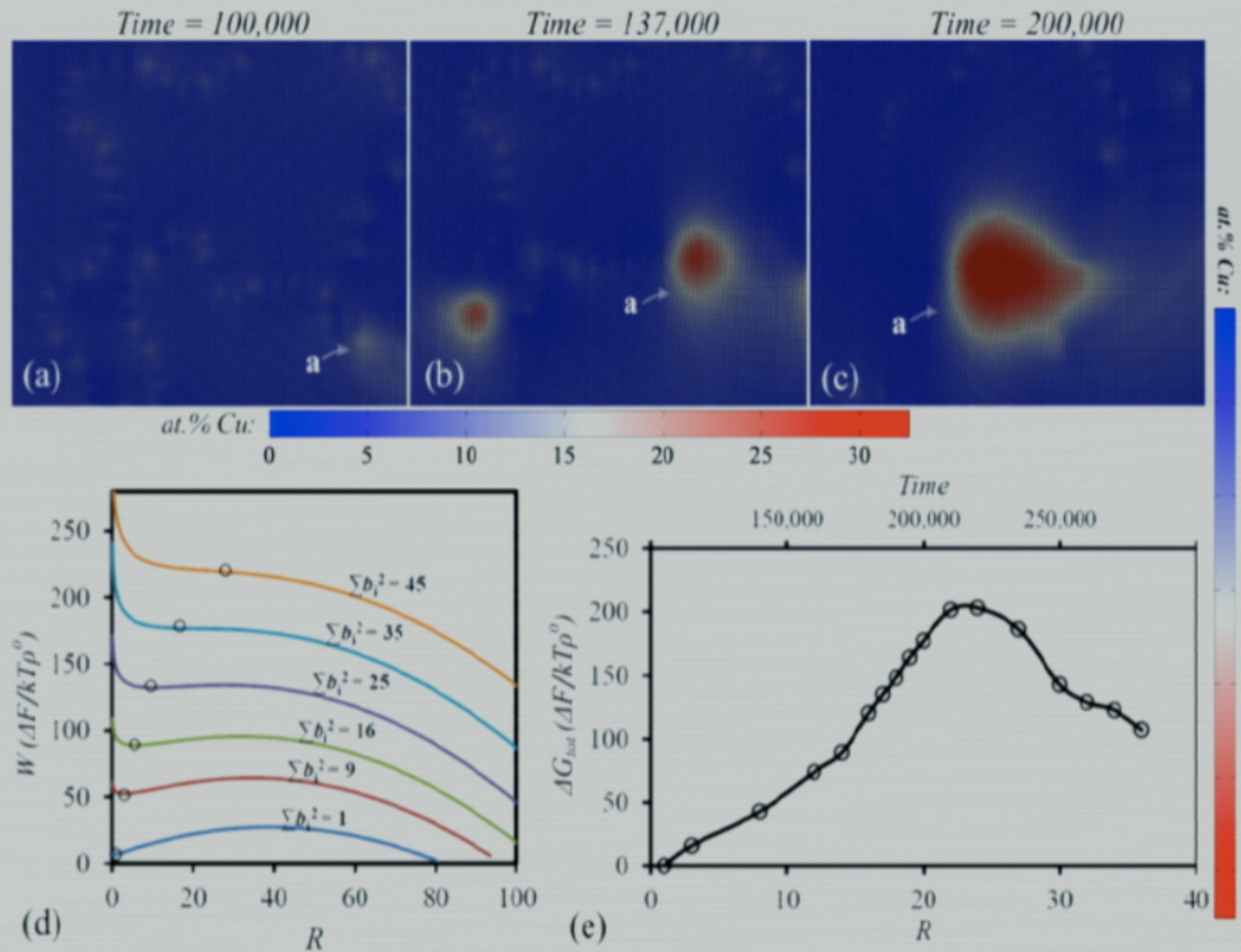

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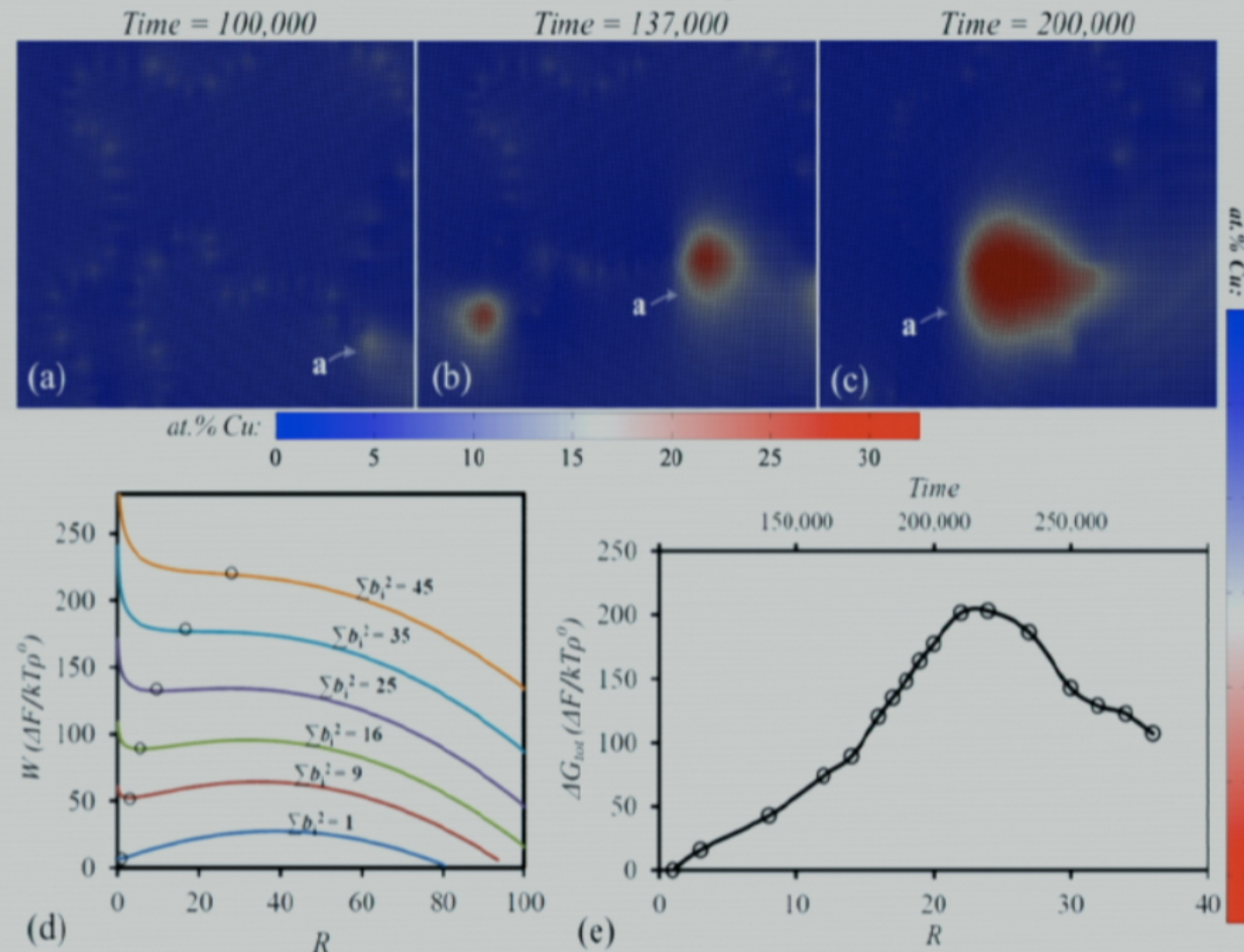
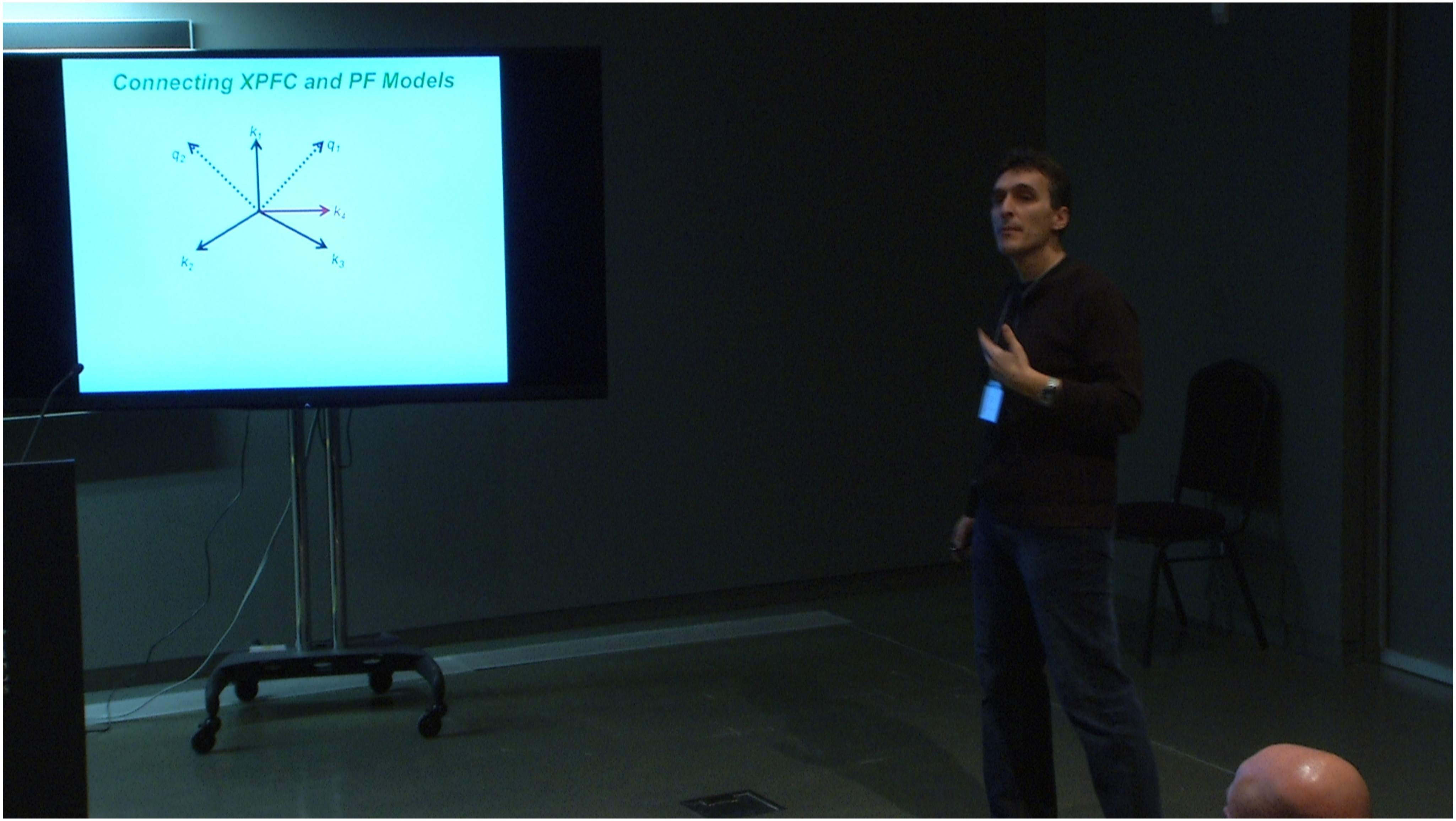
Role of Dislocations on Precipitation

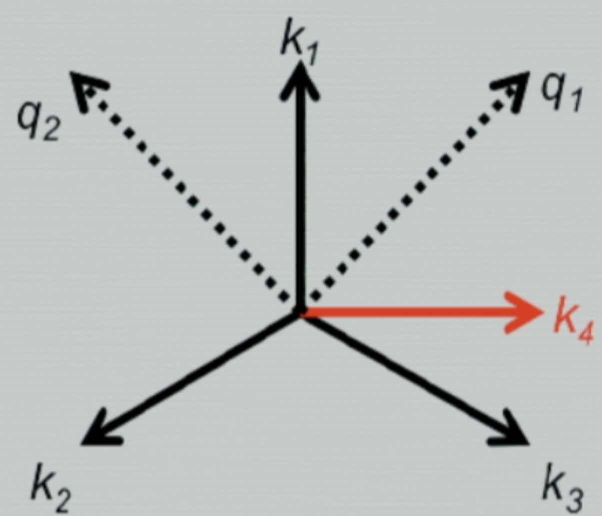


[Vahid Fallah, et. Al Phys. Rev B, 86, 134112 (2012); Acta. Mat., 61, 6372 (2013)]

Connecting XPFC and PF Models


Connecting XPFC and PF Models
k_1
q_2
q_1
k_4
k_2
k_3

Connecting XPFC and PF Models



$$C_2(|\mathbf{r}-\mathbf{r}'|) = \int d\mathbf{k}\, \hat{C}_2(|\mathbf{k}|) e^{\mathbf{i}\mathbf{k}\cdot\mathbf{r}} e^{-\mathbf{i}\mathbf{k}\cdot\mathbf{r}'} \qquad \sum_{l=0}^{\infty} \frac{(-1)^l}{l!} (\mathbf{k}^2)^l \frac{\partial^l \hat{C}_2}{\partial(\mathbf{k}^2)^l}\bigg|_{\mathbf{k}=0}$$

$$n(\mathbf{r}) = n_o(\mathbf{r}) + \sum_j^6 A_j(\mathbf{r}) e^{i\mathbf{k}_j\cdot\mathbf{r}} + \sum_m^6 B_m(\mathbf{r}) e^{i\mathbf{q}_m\cdot\mathbf{r}} + c.c.,$$

Connecting XPFC and PF Models

$$\frac{F}{k_B T \rho_o V} = \int d\mathbf{r} \Bigg\{ \frac{n_o^2}{2} - \eta \frac{n_o^3}{6} + \chi \frac{n_o^4}{12} + \left(1 - \eta n_o + \chi n_o^2\right) \left(\sum_m^4 |A_m|^2 + \sum_m^2 |B_m|^2 \right)$$

$$- (\eta - 2\chi n_o) \left[\left(\prod_m^3 A_m + \text{c.c} \right) + \left(A_1^* A_4^* B_2^* + A_1 A_4^* B_1^* + \text{c.c} \right) \right]$$

$$+ \frac{\chi}{2} \left[\sum_m^4 A_m^2 (A_m^*)^2 + \sum_m^2 B_m^2 (B_m^*)^2 + 4 \left(\sum_m^4 \sum_{j>m}^4 |A_m|^2 |A_j|^2 + \sum_m^4 \sum_j^2 |A_m|^2 |B_j|^2 + |B_1|^2 |B_2|^2 \right) \right]$$

$$+ \chi \left[2A_2^* A_3^* A_4^* B_1^* + 2A_2 A_3 A_4^* B_2^* + A_1^2 B_1^* B_2 + A_4^2 B_1 B_2 + \text{c.c} \right] - \frac{n_o^2}{2} \hat{C}_2(|\mathbf{k}_0|)$$

$$- \frac{1}{2} \sum_m A_m^*(\mathbf{r}) \left[\hat{C}_2(|\mathbf{k} + \mathbf{k}_m|) \hat{A}_m(\mathbf{k}) \right]_{\mathbf{r}} - \frac{1}{2} \sum_m A_m(\mathbf{r}) \left[\hat{C}_2(|\mathbf{k} + \mathbf{k}_m|) \hat{A}_m(-\mathbf{k}) \right]_{\mathbf{r}}$$

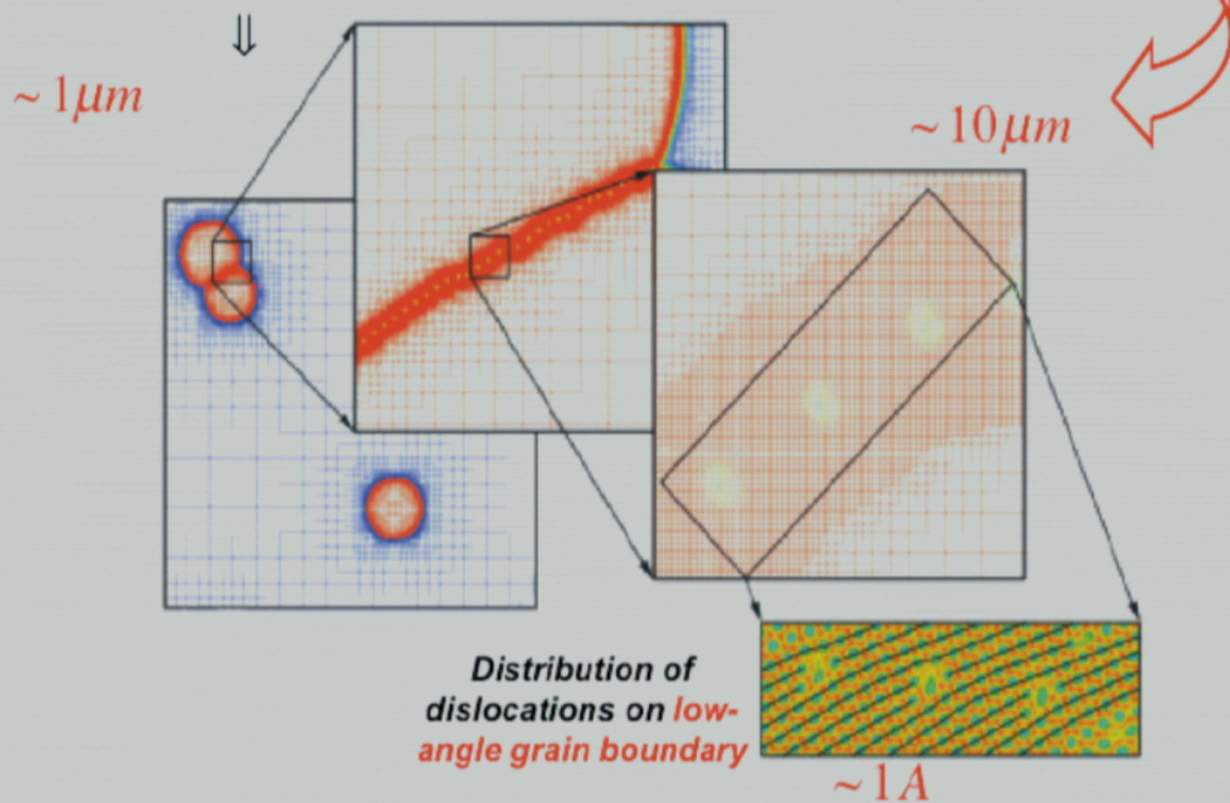
$$- \frac{1}{2} \sum_m B_m^*(\mathbf{r}) \left[\hat{C}_2(|\mathbf{k} + \mathbf{q}_m|) \hat{B}_m(\mathbf{k}) \right]_{\mathbf{r}} - \frac{1}{2} \sum_m B_m(\mathbf{r}) \left[\hat{C}_2(|\mathbf{k} + \mathbf{q}_m|) \hat{B}_m(-\mathbf{k}) \right]_{\mathbf{r}} \Bigg\}$$

$$n(\mathbf{r}) = n_o(\mathbf{r}) + \sum_j^6 A_j(\mathbf{r}) e^{i\mathbf{k}_j \cdot \mathbf{r}} + \sum_m^6 B_m(\mathbf{r}) e^{i\mathbf{q}_m \cdot \mathbf{r}} + c.c.,$$

N. Ofori-Opoku, J. Stolle, Z.F. Huang and N. Provatas, PRB, 88, 104106 (2013)

Density Amplitudes & Adaptive Mesh Refinement

$$\rho(\vec{r},t) = \bar{\rho} + \sum_n \underbrace{\left(\phi_n(\vec{r})\mathrm{e}^{i\theta_n(\vec{r})}\right)}_{A_n}\mathrm{e}^{\vec{K}_n\cdot\vec{r}} \rightarrow S\cdot F\left[\rho(\vec{r})\right] \rightarrow F_{CG}\left[\phi_n,\theta_n\right]$$



[B. Athreya, N. Goldenfeld, J. Dantzig, M. Greenwood N. Provatas, Phys. Rev. E, vol 76 (2007)]