Physics of MRF Regularization for Segmentation of Materials Microstructure Images

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Electronic Imaging for Microscopy-2005 to Date

Incorporate and adapt modern imaging methods for analysis of microscope data

Materials
Marc De Graef (CMU)
Craig Przybyla,
Lawrence Drummy,
Jeff Simmons (AFRL)

EE/Comp. Sci
Charles Bouman, Mary Comer,
Ilya Pollak (Purdue)
Alfred Hero (U. Mich)
Song Wong (U. South Carolina)
Russel Hardie (U. Dayton)

Bayesian Segmentation
(EM/MPM)
Comer

Graphcut Segmentation
(topology preserving)
Wong

Dictionary matching segmentation
(matching persuits)
Pollak

Stabilized inverse diffusion (discontinuities)
(SIDE)
Pollak

Dictionary-based inversion
(EBSD)
Hero

Anomaly detection
(automatic classification of EBSD
Irregular features in large datasets)
Hero, Hardie

Feature Extraction
(velocity gradient
moment invariant texture classifications)
Przybyla, De Graef

TEM Tomographic reconstruction
(HAADF STEM, bright field TEM)
Drummy, Bouman

...always outdated

Opportunity: Co-Evolution of the Ising Model

Physics

Statistical Mechanics

- **Ising (1924)**
  1-D Ising Ferromagnet model
- **Onsager (1944)**
  2-D Ising Ferromagnet model
- **Potts (1952)**
  Extension to multiple spin states

Regularization

- **Hammersley&Clifford(1971)**
  general method for MRF priors
- **Besag (1974)**
  proof of H-C theorem
- **German and German(1984)**
  MC/MC MAP est.
- **Marroquin, et al. (1987)**
  Gibbs Sampler MPM

Statistics/Imaging

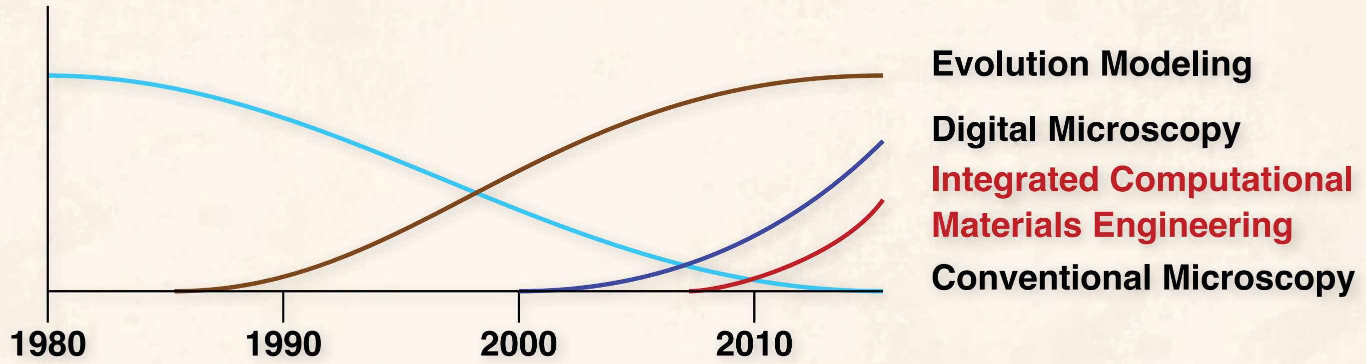
Evolution

- **Binder (1968)**
  Metropolis M/C-thermodynamics
- **Liebowitz, et al. (1976)**
  Ising spin systems
- **Srolovitz, Rollett, Holm, et al. (1988)**
  Evolution of poly-crystalline mat'ls
- **Miodownik, et al. (2000)**
  second phase pinning

Materials

Motivation

Research Trends



Opportunity — **Fusion of evolution modeling with digital microscopy**

parameter estimation for evolution models
physics-based regularization for image analysis

Presentation Goals

Show where MRF regularization ⇔ real material behavior
Uncover unexploited materials properties implicit in MRF

Outline

Motivation — **Integration of techniques**
Legacy: evolution models
Emerging: digital microsopy

Methods — **EM/MPM regularized segmentation**
Physics-dominated extreme

Surface Science — **`Energy penalty' ⇒ `interfacial energy'**
Coarse graining

Physics in MRF Segmentations — **Materials physics intrinsic in MRF regularization**
Commonly observed phenomena
Qualitative

Potential Developments — **Physics not in conventional MRF regularization**
Materials specific extensions

Conclusions

Methods

EM/MPM Segmentation

Comer and Delp, (2000)

Forward model

mixture of Gaussians
EM algorithm for fitting histogram

$$f_{Y|X}(y|x,\theta) = \prod_{r=1}^{N} \frac{1}{\sqrt{2\pi\sigma_{x_r}^2}} \exp\left(-\frac{(y_r - \mu_{x_r})^2}{2\sigma_{x_r}^2}\right)$$

Regularization

4-neighbor MRF

$$p_X(x) = \frac{1}{z} \exp\left(-\sum_{\{r,s\}\in C} \beta_{x_r,x_s}(1 - \delta_{x_r,x_s})\right)$$

δ_{ij} = *Kronekar delta*
C = *4-neighbor clique*

Estimation of posterior marginals

Markov chain Monte Carlo

Phantoms

Slight composition gradients + Poisson noise

artifact boundaries: pure physics

Extremes of Regularization

100% Observation ⟷ **Regularization** ⟷ **100% Physics**

Strong Regularization

Large hyperparameter

Low contrast

Regularization Dominated Segmentation

Gradient + Poisson noise

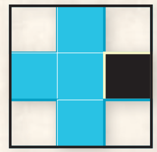
Segmentation

histogram model

Artifact boundary (mixture of Gaussians model)

Surface Science 101 1/2: Coarse Graining

Markov Random Field (p_X)



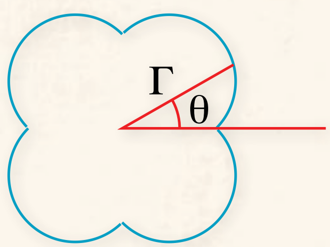
$$1/z \; exp \left[-\sum_{ij} \beta^{\alpha\beta} (1 - \delta^{\alpha\beta}_{ij}) \right]$$

Smoothing:

penalty unless both pixels are same class

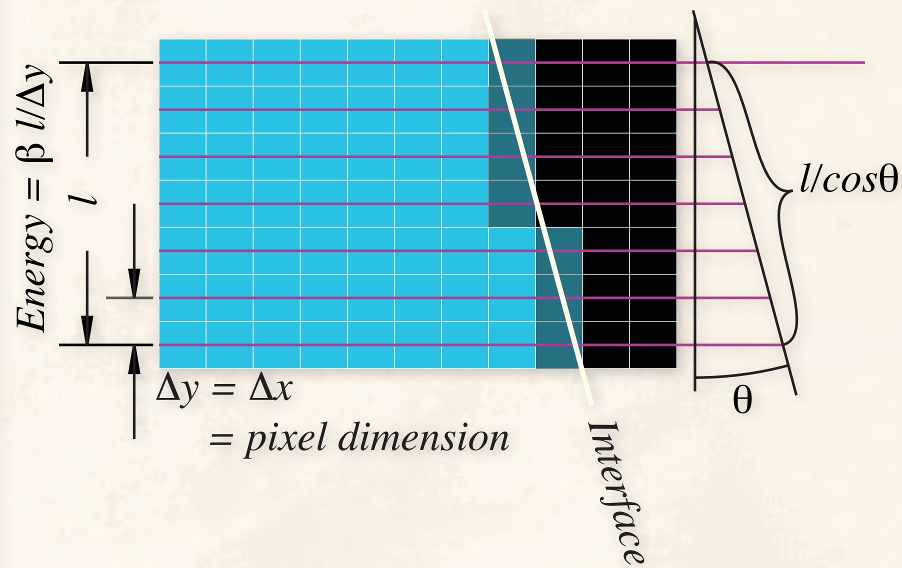
$\beta^{\alpha\beta}$ spatial interaction parameters dependent on classes involved

Anisotropic interface energy density



Wulff plot for 4-neighbor interfacial energy

Coarse-Graining: $\beta \rightarrow \Gamma$



Energy density: horizontal

$(\beta/\Delta y) \cos\theta$

Energy density: vertical

$(\beta/\Delta x) \sin\theta$

Total interfacial energy density

$\Gamma_{0°K} = \sqrt{2}(\beta/\Delta y) \sin(\theta + \pi/4) \qquad \theta \in [\, 0, \pi/2 \,]$

Surface Science 101 2/2: Interface `Tension’

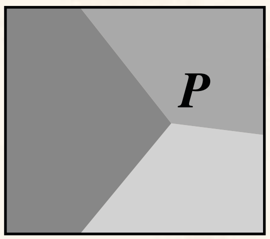
`Energy’ $\Rightarrow$ `force’

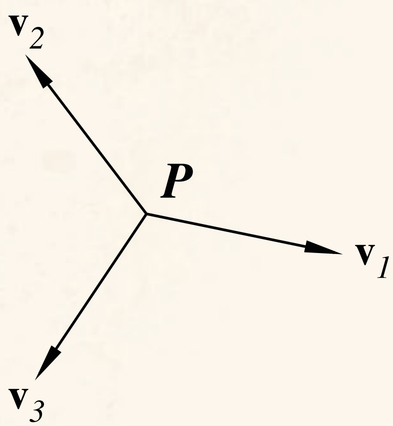
Regularizing boundary with `energy’

$\Rightarrow E(\mathbf{P})$

$\Rightarrow \mathbf{F} = \nabla E(\mathbf{P})$

$\mathit{Equilibrium} \Rightarrow \mathbf{F} = 0$





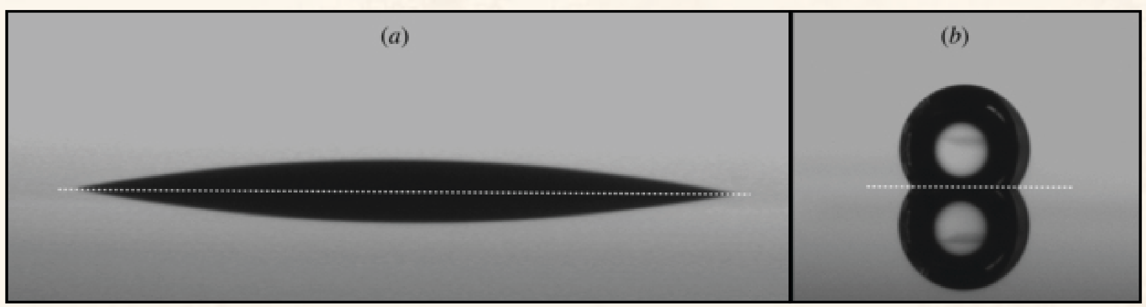
$$\sum_i \Gamma_i \mathbf{v}_i = 0$$

$\mathbf{v}_i$ = *vector from P in direction of boundary*

$$\Gamma_i \triangleq \left| \frac{dE_i}{d\mathbf{v}_i} \right|$$

Example

Fig. 6 of Gari Arutinov, et al., J. Micromech. Microeng., 22, 115022, (2012).



Oxidized SiO_2 substrate — *Gold coated SiO_2 substrate*

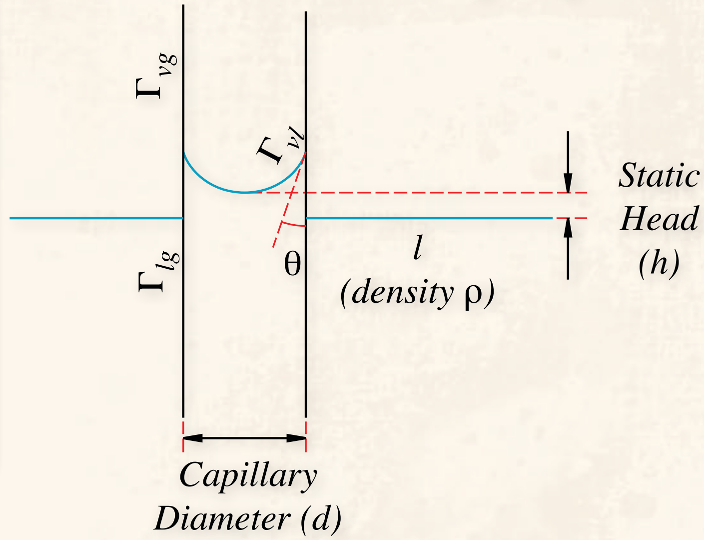
Surf. Sci. in MRF-Regularized Segmentations

Capillarity	**Surface energy induced lifting of one phase** *extending region with interface length penalty*
Wetting	**Coating phases with `boundary phase'** *thin region separating two larger regions of different classes*
Pinning	**Pinning** *interaction of boundaries with regions*

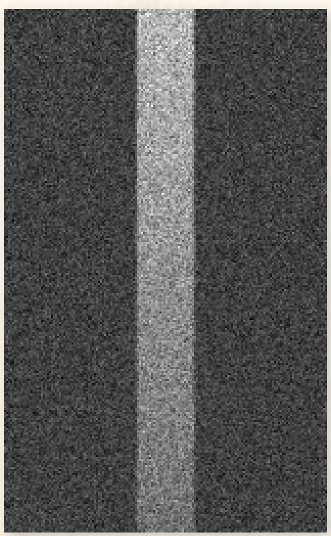
Capillarity Lifting

Physics

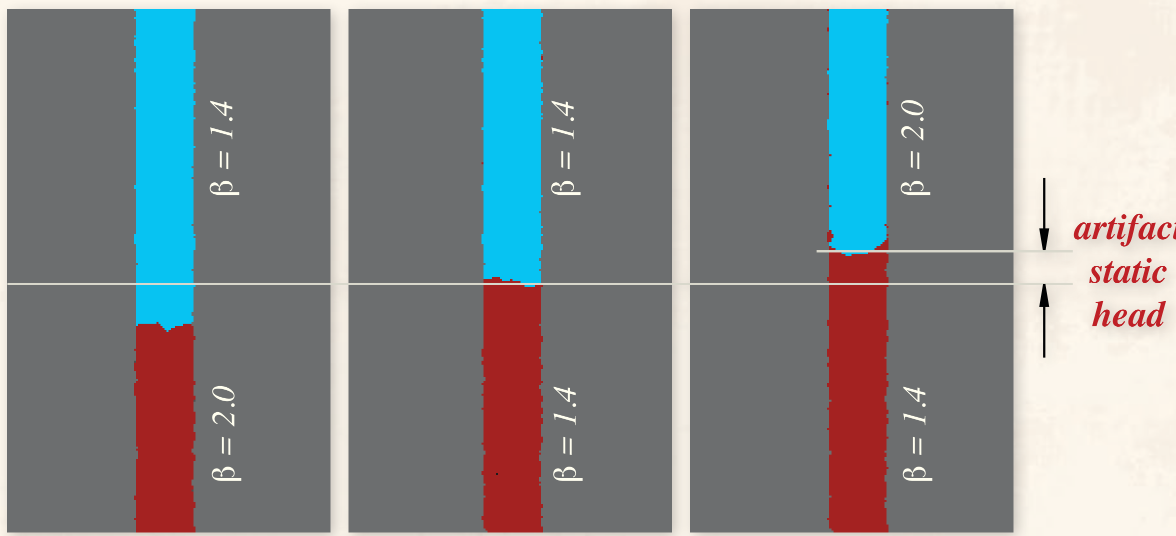
$$\rho = 2(\Gamma_{vg} - \Gamma_{lg} - \Gamma_{vl} \cos\theta)/dh$$



Regularized Segmentation



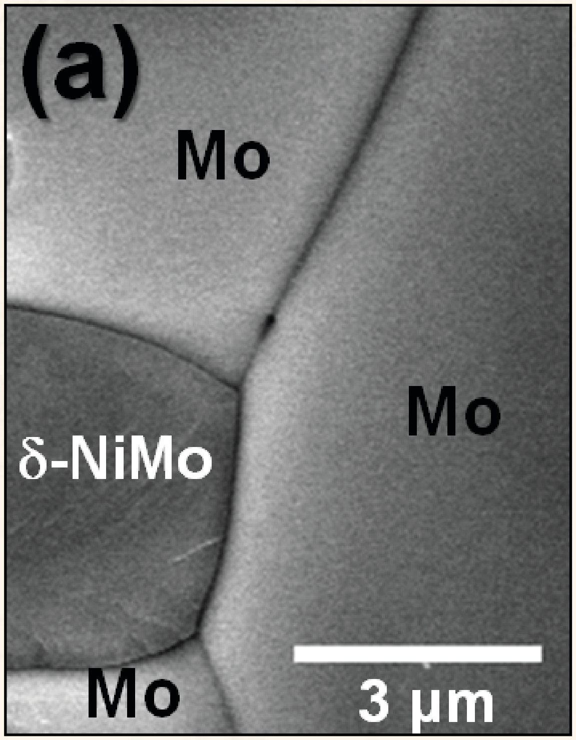
Phantom



Wetting

Mo grains at two different temperatures

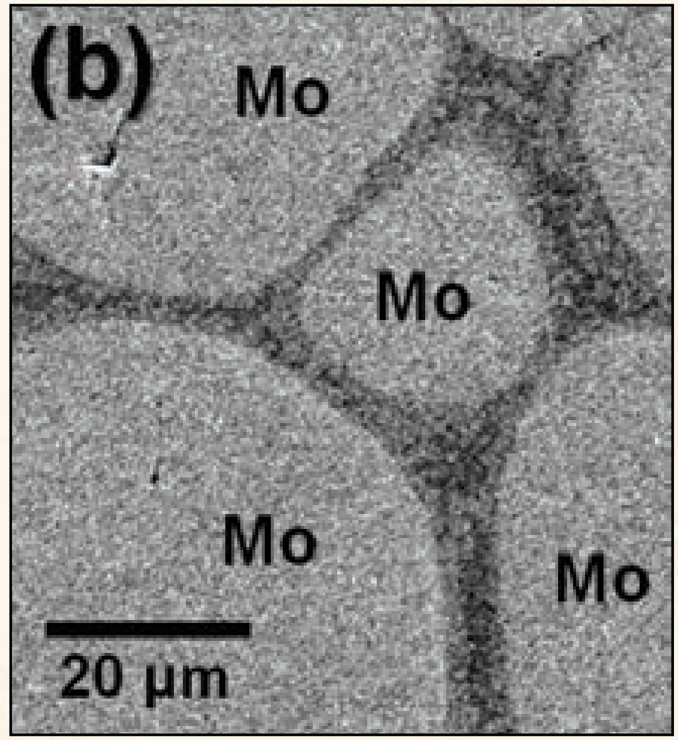
interfacial energy fn of temperature



Non-wet interfaces

SEM image

Mo-12.4%Ni quenched from 1344C



Wet interfaces

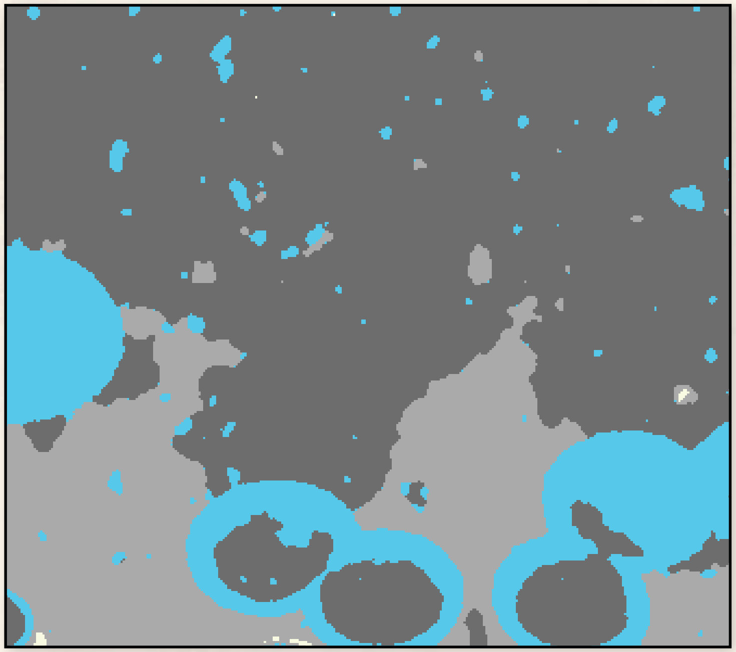
Cross-sectional SEM image

Mo-12.4%Ni quenched from 1495C

Courtesy Jian Luo

Xiaomeng Shi and Jian Luo, Appl. Phys. Lett., 94, 251 908, (2009)

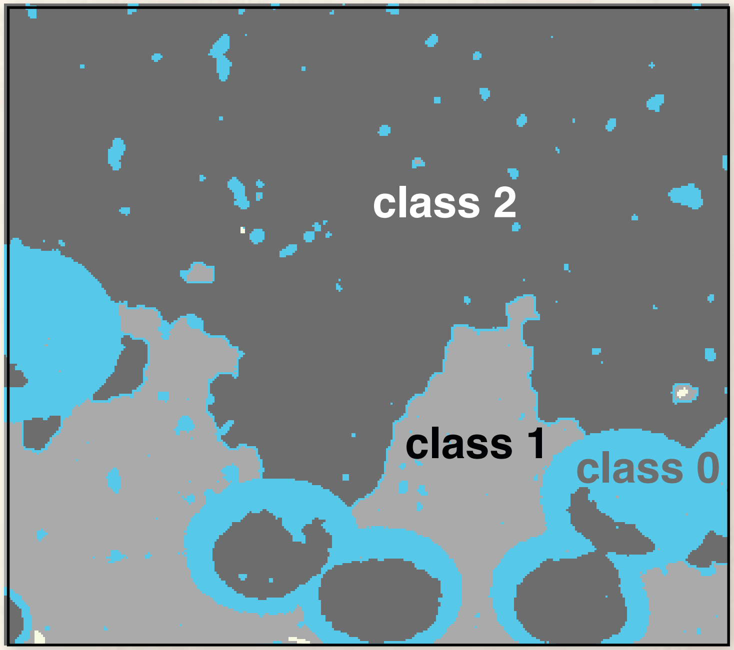
Thin Region Separating Two Regions



Segmented image

$\beta_{0,1}=0.9$, $\beta_{0,2}=\mathbf{0.5}$, $\beta_{1,2}=\mathbf{0.9}$

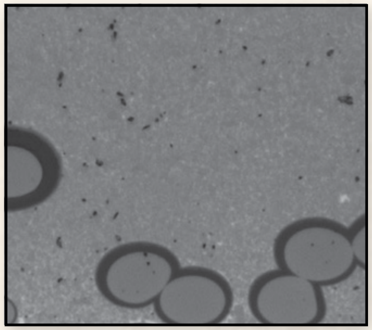
non-wet interface



Segmented image

$\beta_{0,1}=0.9$, $\beta_{0,2}=\mathbf{0.9}$, $\beta_{1,2}=\mathbf{1.8}$

wet interface



Raw image

SiC fiber in SiC matrix. BN coating

Imaging:

optical

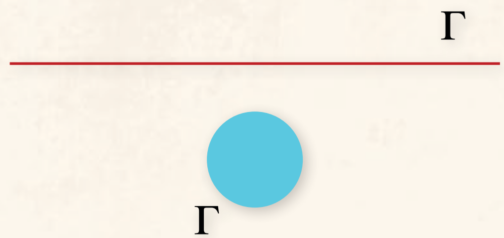
slight intensity gradient in BG

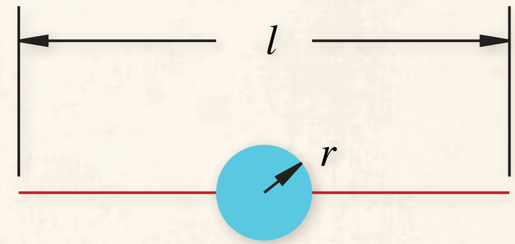
Ex 2: Zener Pinning for Grain Refinement

Friction Force

Interface `attracted to' particles

Reduces boundary penalty





$E = 2\pi\, r\, \Gamma + l\, \Gamma$

$E = 2\,\pi\, r\, \Gamma + l\, \Gamma - 2r\, \Gamma$

`Friction force' of $2r\Gamma$ pinning the boundary

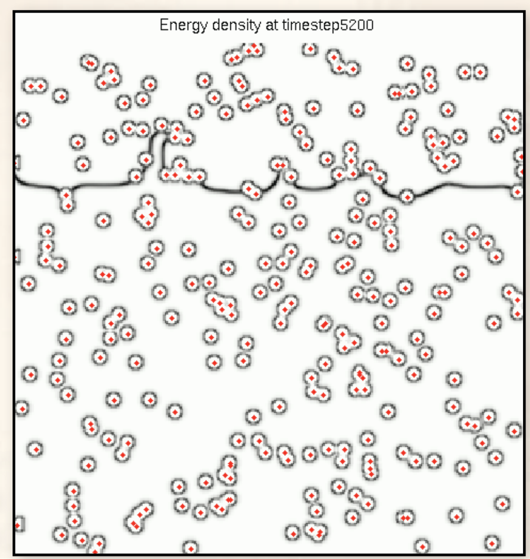
Zener Pinning Mechanism

Zener, unpublished
(cited C.S. Smith, 1948)

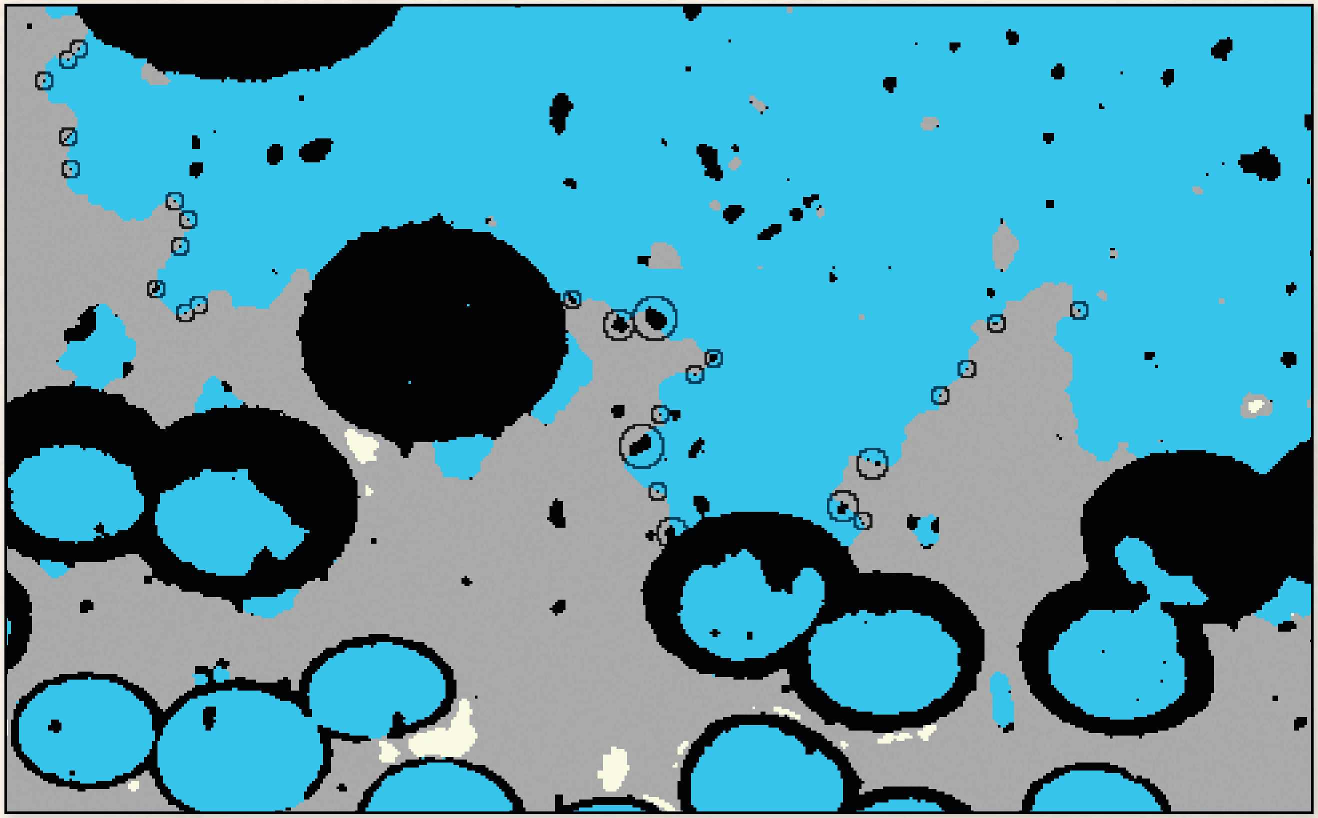
Used in alloy design

stop grains from growing

Source:
commons.wikimedia.com
(Zener Pinning)



Interaction of Boundaries with Regions



Individual particles in image `pin' boundary

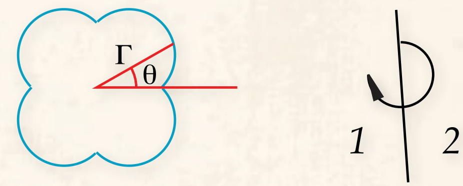
Boundary intersects large black classes at right angles

Future Materials-Specific Extensions

Anisotropic interfacial energy

cusps imply torques

8-neighbor has cusps in [1 1] directions



Coarse graining: quantitative link to materials

Γ can be estimated from β with Monte Carlo (Binder)

Requires a `temperature' of the MRF

Thermodynamics

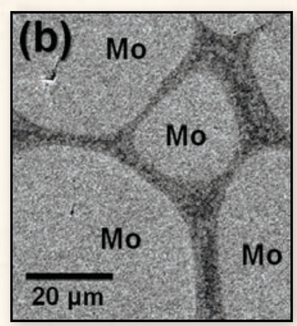
$$F = E - T\,H$$

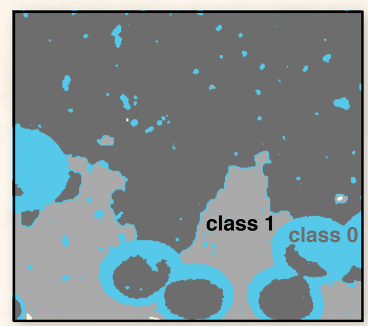
Statistical Mechanics

$$T = \frac{RMS(E)}{k_b N c_v}$$

Wetting: potential robust segmentation

experiment: ***boundries between same classes***





Conclusions

MRF is a generalization of Ising Model

solid state physics

Reproduces classical surface science

qualitative

Materials-specific extensions possible

Ising model reflects actual materials behavior

Expected uses

inpainting
boundary orientations
quatititative regularization
separation of spatially close regions in segmentations