Physics of MRF Regularization for Segmentation of Materials Microstructure Images

Jeff Simmons†
Craig Przybyla†
Stephen Bricker‡
Dae Woo Kim*
Mary Comer*

†Materials and Manufacturing Directorate; Air Force Research Laboratory; OH 45433; USA
‡Department of Electrical and Computer Engineering; University of Dayton; OH 45469; USA
*Department of Electrical and Computer Engineering; Purdue University; IN 47907
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 pursuits)
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

**Stabilized inverse diffusion (discontinuities)**
(SIDE)
Pollak

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

...always outdated
Opportunity: Co-Evolution of the Ising Model

Physics

- **Ising (1924)**
  1-D Ising Ferromagnet model

- **Onsager (1944)**
  2-D Ising Ferromagnet model

- **Potts (1952)**
  Extension to multiple spin states

Statistical Mechanics

- **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

Statistics/Imaging

- **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

Materials
Motivation

Research Trends

Evolution Modeling
Digital Microscopy
Integrated Computational Materials Engineering
Conventional Microscopy

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 $\iff$ real material behavior
Uncover unexploited materials properties implicit in MRF
Outline

Motivation
Integration of techniques
  Legacy: evolution models
  Emerging: digital microscopy

Methods
EM/MPM regularized segmentation
  Physics-dominated extreme

Surface Science
`Energy penalty’ ⇒ `interfacial energy’
  Coarse graining

Physics in MRF Segments
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**

- Forward model
  - mixture of Gaussians
  - EM algorithm for fitting histogram

**Comer and Delp, (2000)**

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

**Regularization**

- **4-neighbor MRF**

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

\[\delta_{ij} = \text{Kronekar delta}\]

- \(C = 4\text{-neighbor clique}\)

**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)
Markov Random Field (pX)

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

Smoothing:
penalty unless both pixels are same class
\(\beta^{\alpha \beta}\) spatial interaction parameters
dependent on classes involved

Anisotropic interface energy density

\[\Gamma_{0^\circ K} = \sqrt{2} \frac{\beta \Delta y}{\Delta y} \sin(\theta + \pi / 4) \quad \theta \in [0, \pi / 2]\]

Coarse-Graining: \(\beta \rightarrow \Gamma\)

Energy density: horizontal
\((\beta / \Delta y) \cos \theta\)

Energy density: vertical
\((\beta / \Delta x) \sin \theta\)

Wulff plot for 4-neighbor interfacial energy

Smoothing:
penalty unless both pixels are same class
\(\beta^{\alpha \beta}\) spatial interaction parameters
dependent on classes involved
`Energy’ ⇒ `force’

Regularizing boundary with `energy’

⇒ $E(P)$
⇒ $F = \nabla E(P)$

Equilibrium ⇒ $F = 0$

$\sum_i \Gamma_i v_i = 0$

$v_i = \text{vector from } P\text{ in direction of boundary}$

$\Gamma_i \triangleq \left| \frac{dE_i}{d\nu_i} \right|$}

Example

Fig. 6 of
Gari Arutinov, et al.,

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

\[ \beta = 1.4 \]

\[ \beta = 2.0 \]

\[ \rho = 2 \left( \Gamma_{vg} - \Gamma_{lg} \cdot \Gamma_{vl} \cos \theta \right) / dh \]

Physics

Regularized Segmentation

Phantom

\[ \text{Capillary Diameter (d)} \]

\[ \text{Static Head (h)} \]

\[ \Gamma_{vg} \]

\[ \Gamma_{lg} \]

\[ \Gamma_{vl} \]

\[ \theta \]

\[ l \]

\[ \text{artifact static head} \]
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

Thin Region Separating Two Regions

Segmented image
\[ \beta_{0,1}=0.9, \beta_{0,2}=0.5, \beta_{1,2}=0.9 \]
non-wet interface

Segmented image
\[ \beta_{0,1}=0.9, \beta_{0,2}=0.9, \beta_{1,2}=1.8 \]
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**

*Used in alloy design*

*stop grains from growing*

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

**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*
- $\Gamma$ can be estimated from $\beta$ with Monte Carlo (Binder)
- Requires a `temperature’ of the MRF

**Thermodynamics**
$$F = E - T H$$

**Statistical Mechanics**
$$T = \frac{\text{RMS}(E)}{k_b N c_v}$$

**Wetting:** *potential robust segmentation*
- *experiment: boundaries 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
- quantitative regularization
- separation of spatially close regions in segmentations