Heterogeneity and Phase Transformations in Ferroelastics: From JAK to Now.

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### JAK with G. Barsch: Nonlinear Physics of Materials

Free energy (C-T), FePd, 1D solutions '84; Decaying fringing fields in austenite '87; Tweed as spin glass' 91; Shuffle order parameter '94; Strain compatibility, tweed ' 95 ;



S. Kartha et al, PRL 67, 3630 (1991).





#### OUTLINE

• Linear vs. Nonlinear Elasticity in Strain

(.. and rotation)



 $Pb_3(VO_3)_2$ 

Glass Martensite: Continuum to Discrete Models
 (MC, Mean Field Theory, RG)

: Transition from Martensite to Glass

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**Ferroic:** "crystal with two or more distinct orientation states and switching between them by external fields" (Aizu, 69)

Multiferroic: two or more coexisting ferroic properties in the same phase

Ferromagnetic Ferroelectric Ferroelastic Ferrotoroidal, ....



### Ferroelastics

• Elastic heterogeneities: habit planes, twin boundaries :polydomains (aggregates)

Issues: orientations, specific microstructure,.... (Wechsler-Liebermann-Read, Bowles McKenzie, Eshelby, Sapriel, Roytburd, Khachaturyan,.....)





### SYMMETRY ADAPTED STRAINS FOR CUBIC SYSTEM







• Elastic constants



Sato, 91



### **ENERGY MINIMIZATION: Solve for displacement fields**

Monte Carlo:
$$\mathcal{U}_x, \mathcal{U}_y$$
Kartha et al., 95Relaxation, steepest descent: $\mathcal{U}_x, \mathcal{U}_y$ Jacobs, 85, 92Newton's equations: $\mathcal{U}_x, \mathcal{U}_y, \mathcal{U}_z$ Ahluwalia et al., 06 $\rho \vec{\vec{u}} = \vec{\nabla} \cdot \vec{\sigma}_{elastic} + \vec{\nabla} \cdot \vec{\sigma}_{dissipative}$  $\mathcal{R} = \int d\vec{r} \mathbf{A}_1' \dot{\varepsilon}_{ij} \dot{\varepsilon}_{kl}$  $\sigma_{ij}^{elastic} = \frac{\delta F}{\delta \varepsilon_{ij}}$  $\sigma_{ij}^{dissipative} = \frac{\delta R}{\delta \dot{\varepsilon}_{ij}}$  $R = \int d\vec{r} \mathbf{A}_1' \dot{\varepsilon}_{ij} \dot{\varepsilon}_{kl}$ 







Kartha et al. PRB' 95

### Elastic Signatures in Polarons via single-crystal diffuse scattering













## Solve for equilibrium microstructure using compatibility of strains

A CONTRACT ON A

$$\sigma(x) = C(x) : \varepsilon(x)$$

$$\sigma(x) = C^{0}(x) : \varepsilon(x) + \delta C : \varepsilon(x)$$
Moulinec and Suquet, 94, 98
Moulinec and Suquet, 94, 98
Microstructure'
$$\sigma(x) = C^{0}(x) : \varepsilon(x) + \delta C : \varepsilon(x)$$
Heterogeneous
Microstructure'
Microstructure'
$$\sigma(x) = C^{0}(x) : \varepsilon(x) + \tau(x)$$
Linear problem
$$\varepsilon(u(x)) = \Gamma^{0}(x) * \tau(x)$$

$$\varepsilon(k) = \Gamma^{0}(k) \tau(k)$$

**Iteratively solve for** 

$$\sigma(x), arepsilon(x)$$





### **GEOMETRICAL NONLINEARITY:** linear strains —>displacement gradients

$$\begin{split} F_{ij} &= \frac{\partial x_i}{\partial X_j} = \frac{\partial \left(x_i - X_i + X_i\right)}{\partial X_j} = \frac{\partial \left(u_i + X_i\right)}{\partial X_j} = \delta_{ij} + \frac{\partial u_i}{\partial X_j} \end{split}$$

$$\begin{aligned} \mathsf{G-L}_{\text{strains}} &\epsilon_{ij} = \frac{1}{2} \left(F^T F - I\right) = \frac{1}{2} \left(\frac{\partial u_i}{\partial X_j} + \frac{\partial u_j}{\partial X_i} + \sum_k \frac{\partial u_k}{\partial X_i} \frac{\partial u_k}{\partial X_j}\right) x_i \overset{\bullet}{} \end{split}$$

Displacement gradients 📥 GL strains

$$D_{ij} \equiv \frac{\partial u_i}{\partial X_j} \begin{array}{l} d_1 = \frac{1}{2}(D_{xx} + D_{yy}) \\ d_2 = \frac{1}{2}(D_{xx} - D_{yy}) \\ d_3 = \frac{1}{2}(D_{xy} + D_{yx}) \\ d_4 = \frac{1}{2}(D_{xy} - D_{yx}) \end{array} \begin{array}{l} e_1 = d_1 + \frac{1}{2} \left[ (d_1)^2 + (d_2)^2 + (d_3)^2 + (d_4)^2 \right] \\ e_2 = d_2 + d_1 d_2 - d_3 d_4, \\ e_3 = d_3 + d_1 d_3 + d_2 d_4 \end{array}$$

**Compatibility:** 

$$\frac{\partial D_{xy}}{\partial X} = \frac{\partial D_{xx}}{\partial Y},$$

$$\hat{d}_1 = \frac{k_x^2 - k_y^2}{k_x^2 + k_y^2} \hat{d}_2 + \frac{2k_x k_y}{k_x^2 + k_y^2} \hat{d}_3,$$

$$\hat{d}_4 = \frac{2k_x k_y}{k_x^2 + k_y^2} \hat{d}_2 - \frac{k_x^2 - k_y^2}{k_x^2 + k_y^2} \hat{d}_3.$$

# Steady State shear strain after quench through transition



### Reference

Current

$$e_3 = 1/2(\varepsilon_{xy} + \varepsilon_{yx})$$



Orientation

# **Rotations Follow Strains**



# **Coarsegraining:**









(3+1) clock 0 model n = 1, 2, 3 and 0

# **Other structural transitions:**



Twinned microstructure for cubic to tetragonal from MFT



Vasseur et al. (2010)

Cubic-Tetragonal (N\_v=3)

### Tetragonal-Orthorhombic (N\_v=2)





Cubic-Trigonal (N\_v=4)



Cubic-Orthorhombic (N\_v=6)



$$H = -\sum_{\langle i,j \rangle} J_{ij}(\tau) S_i S_j + \sum_i \Delta_i(\tau) S_i^2 \qquad \qquad \mathcal{P}(J_{ij}) = \frac{1}{\sqrt{2\pi\sigma_j}} \exp\left\{-\frac{[J_{ij} - J_0(\tau)]^2}{2\sigma_j^2}\right\} \\ + \text{long-range} \qquad \qquad \mathcal{P}(\Delta_i) = \frac{1}{\sqrt{2\pi\sigma_\lambda}} \exp\left\{-\frac{[\Delta_i - \Delta_0(\tau)]^2}{2\sigma_\lambda^2}\right\} \\ \frac{\Delta}{2\sigma_\lambda} J \qquad \qquad \text{distributions} \qquad J_o \neq 0 \\ \text{Order Parameters:} \qquad a) \text{ Mean field: Replica} \\ m = \overline{\langle S \rangle} p = \overline{\langle S^2 \rangle} \qquad b) \text{ Monte Carlo} \\ q = \overline{\langle S \rangle^2} \quad \begin{array}{c} \text{Glass phase,} \\ \text{Edwards-Anderson OP} \end{array} \qquad c) \text{ Renormalization Group} \\ \end{array}$$

# Thermodynamic Phases and RG fixed points

| Phase        | OP characterization       | RG fixed point   |
|--------------|---------------------------|--|
| Austenite    | m = q = 0, p small        | $\Delta^* = +\infty, \ J^* = 0, \ \sigma_J^* = 0$                  |
| Martensite   | $m\neq 0,p\neq 0,q\neq 0$ | $\Delta^* = -\infty, \ J^* = \infty, \ \frac{\sigma_J^*}{J^*} = 0$ |
| Tweed        | m = q = 0, p large        | $\Delta^*=-\infty,J^*=0,\sigma_J^*=0$                              |
| Strain glass | $m=0,p\neq 0,q\neq 0$     | $\Delta^*=-\infty,J^*=0,\sigma_J^*=\infty$                         |

$$m = \overline{\langle S \rangle}$$
  $p = \overline{\langle S^2 \rangle}$   $q = \overline{\langle S \rangle^2}$ 

$$\beta H = -\sum_{\langle i,j \rangle} J_{ij}(\tau) S_i S_j + \Delta(\tau) \sum_i S_i^2 - K \sum_{\langle i,j \rangle} S_i^{\overline{2}} S_j^2$$
$$\{ \mathcal{P}'(J'_{ij}), \mathcal{P}'(\Delta'_i), \mathcal{P}'(K'_{ij}) \} = \mathcal{R}\left[ \{ \mathcal{P}(J_{ij}), \mathcal{P}(\Delta_i), \mathcal{P}(K_{ij}) \} \right]$$

# Phase diagram





# Transition from glass to long range ordered martensite phase in $Ti_{50}(Pd_{40}Cr_{10})$ alloy

#### In-situ synchrotron XRD from 400K to 100K



#### In-situ TEM from 400K to 100K



Xue, Zhou et al. (2011)

Interplay of disorder and long-range

$$\beta H = -\sum_{\langle i,j \rangle} J_{ij}(\tau) S_i S_j + \Delta(\tau) \sum_i S_i^2 + \frac{\beta A_1}{2} \sum_{ij} S_i U_{ij} S_j.$$

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### Summary:

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