Physics of Materials

Chapter 3: Theory of Elasticity

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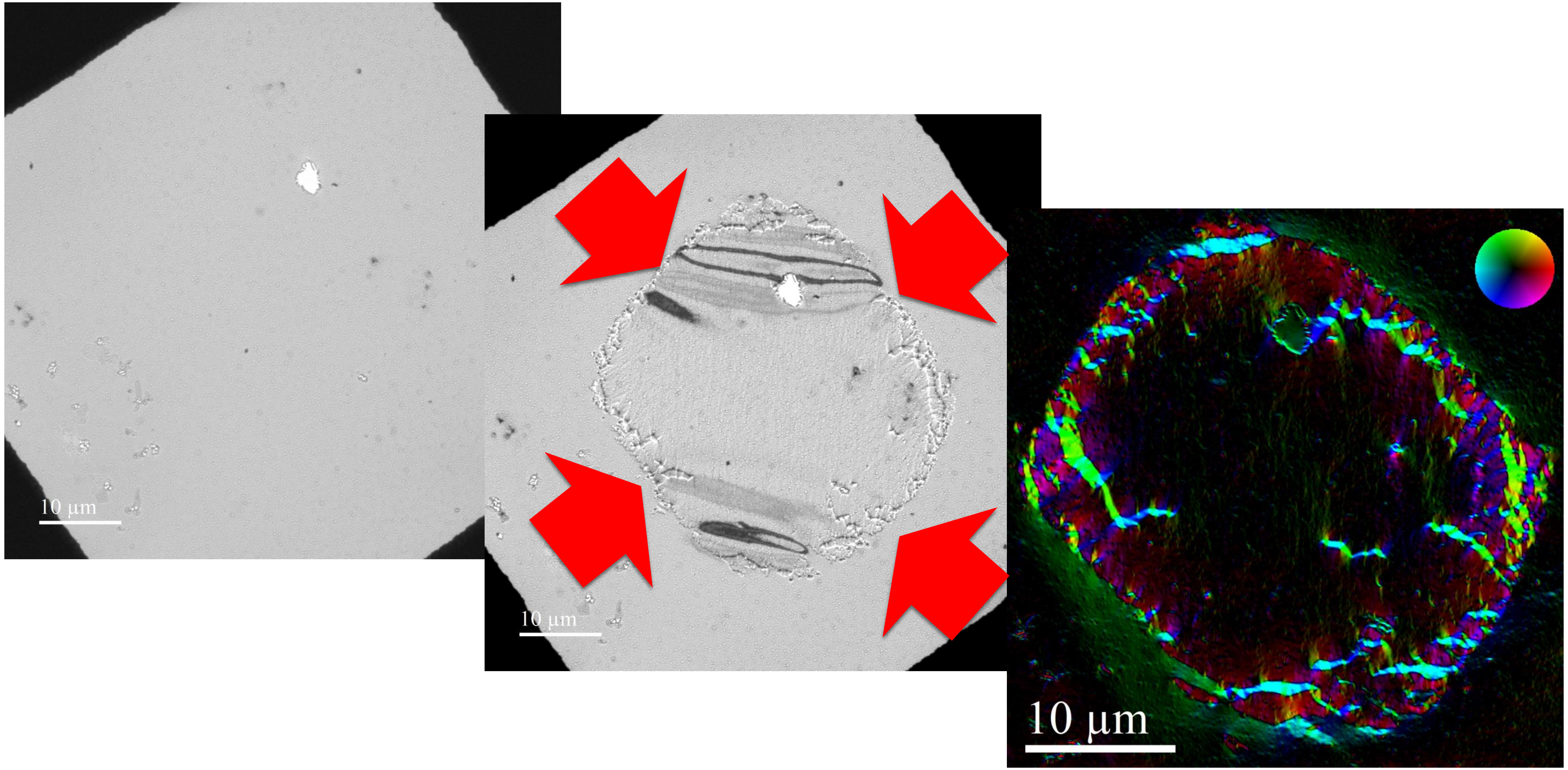
Masters Course PHYS-307

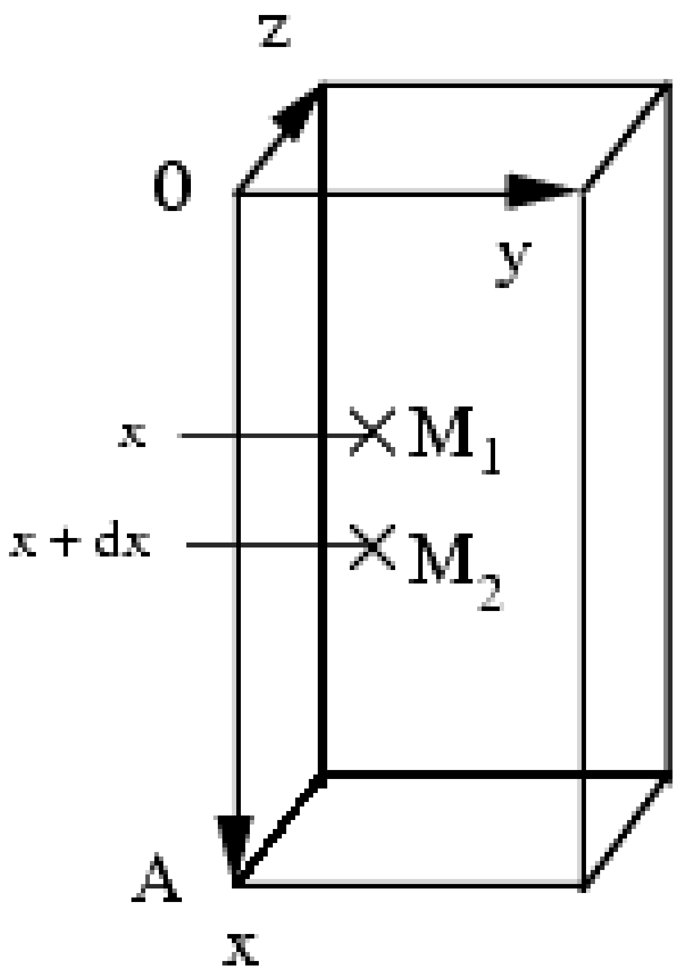
Fall 2024

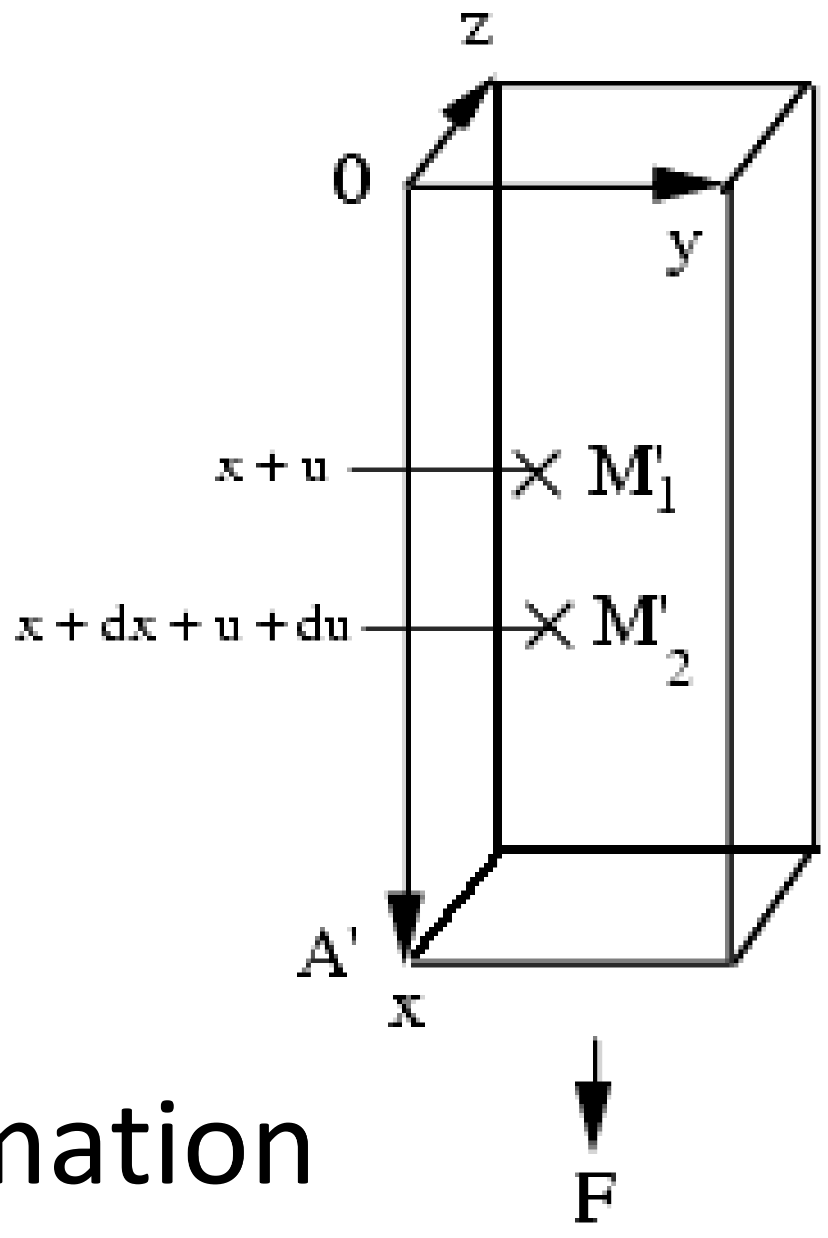
FM transition of FeRh within AFM phase induces elastic stresses



The compressive bi-axial elastic stresses due to the volume expansion accompanying the transition inhibit the ferromagnetic transition and fragments

Simple laws of linear elasticity





Hooke's law

$$\sigma = E \cdot \varepsilon$$

Deformation

$$\varepsilon = \frac{M'_1 M'_2 - M_1 M_2}{M_1 M_2} = \frac{du}{dx}$$

Assumptions

1. Homogenous
2. Isotropic
3. Equilibrium
4. Reversible

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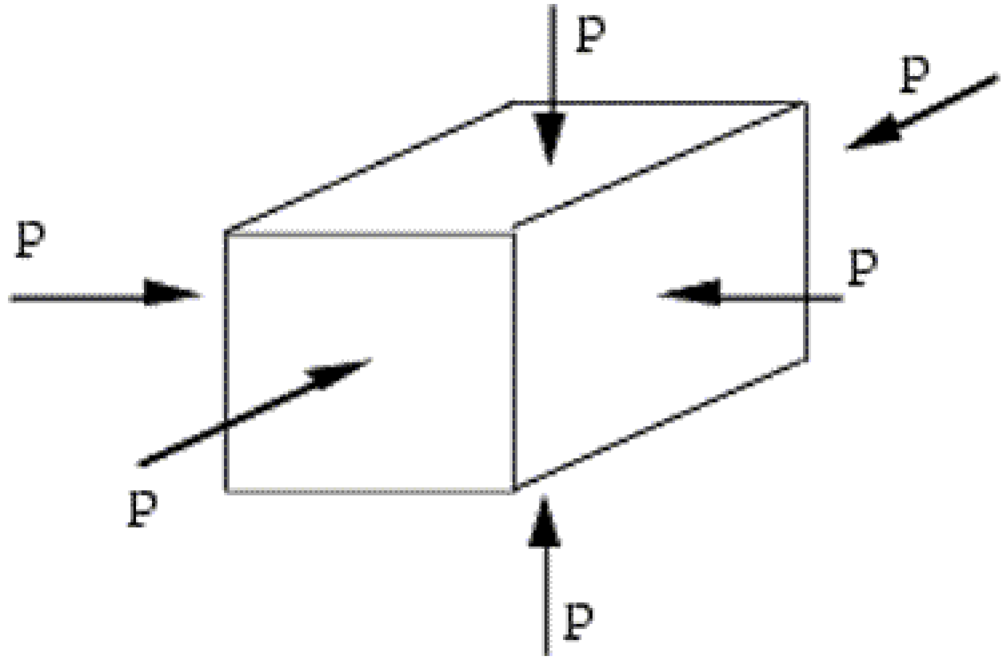
Hooke's law

$$\boxed{\sigma = E \cdot \varepsilon}$$

Example : hydrostatic compression



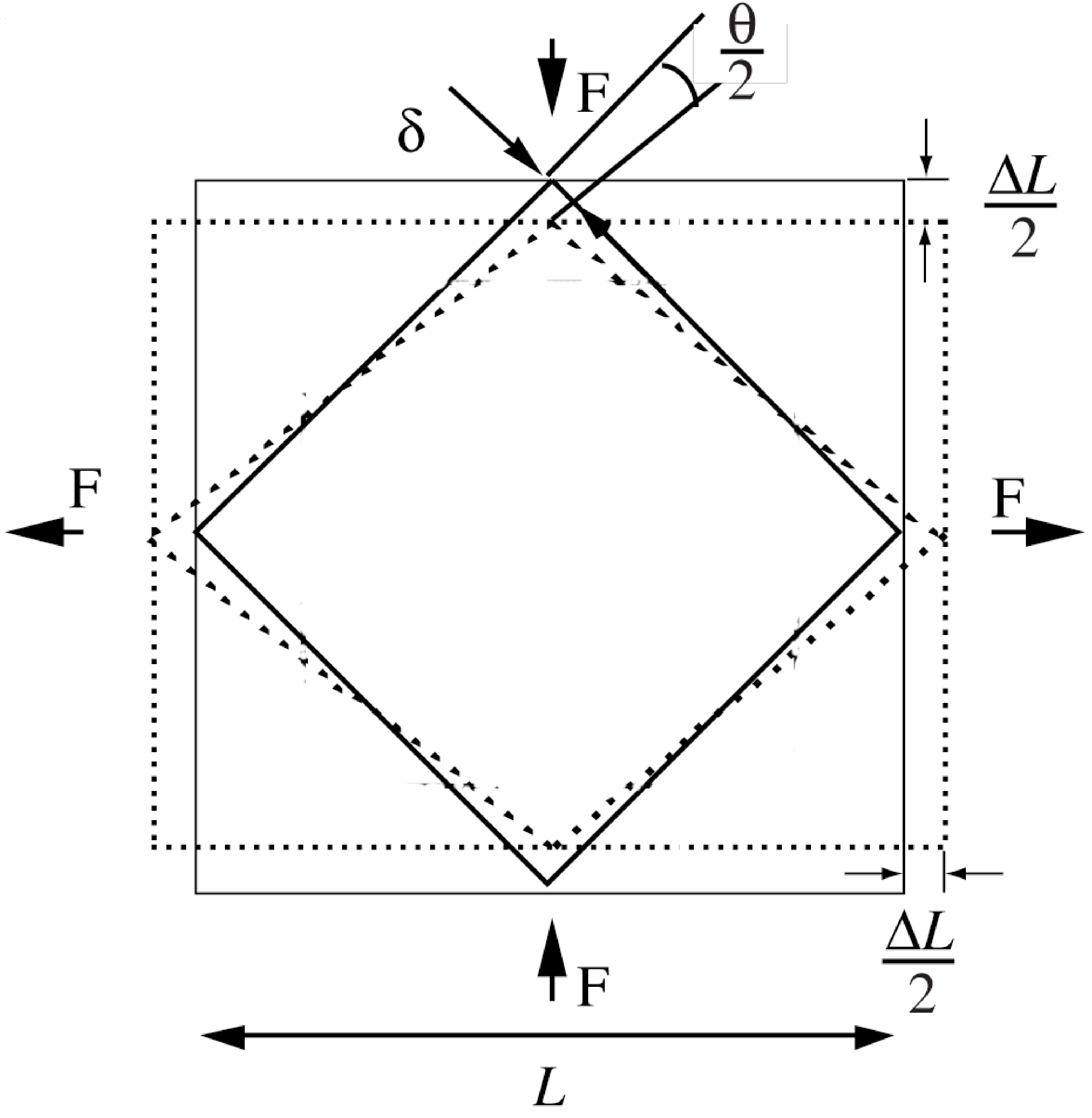
$$\frac{\Delta h}{h} = -\frac{p}{E} + \nu\frac{p}{E} + \nu\frac{p}{E} = -\frac{p}{E}(1-2\nu)$$

$$\frac{\Delta V}{V} = \frac{\Delta h}{h} + \frac{\Delta w}{w} + \frac{\Delta l}{l} = -\frac{3 \cdot p}{E}(1-2\nu)$$

$$p = -K\frac{\Delta V}{V} \qquad K = \frac{E}{3(1-2\nu)}$$

Remember from your introductory thermodynamics course discussing the ideal gas law. K is the compressibility, described as ***K~1/p***

Example: pure shear-stress



$$\frac{\Delta L}{L} = \frac{F}{S}\left(\frac{1+\nu}{E}\right) = \sigma\left(\frac{1+\nu}{E}\right)$$

$$\frac{\Delta L}{2} = \sqrt{2}\cdot\delta = \sqrt{2}\cdot\frac{L}{2}\frac{\sqrt{2}}{2}\sin\frac{\theta}{2} \simeq \theta\frac{L}{4}$$

$$\Rightarrow \frac{\Delta L}{L} = \frac{\theta}{2}$$

$$\theta = 2\sigma\left(\frac{1+\nu}{E}\right)$$

But... $\sigma = \mu\theta$

Shear modulus $\mu = \frac{E}{2(1+\nu)}$

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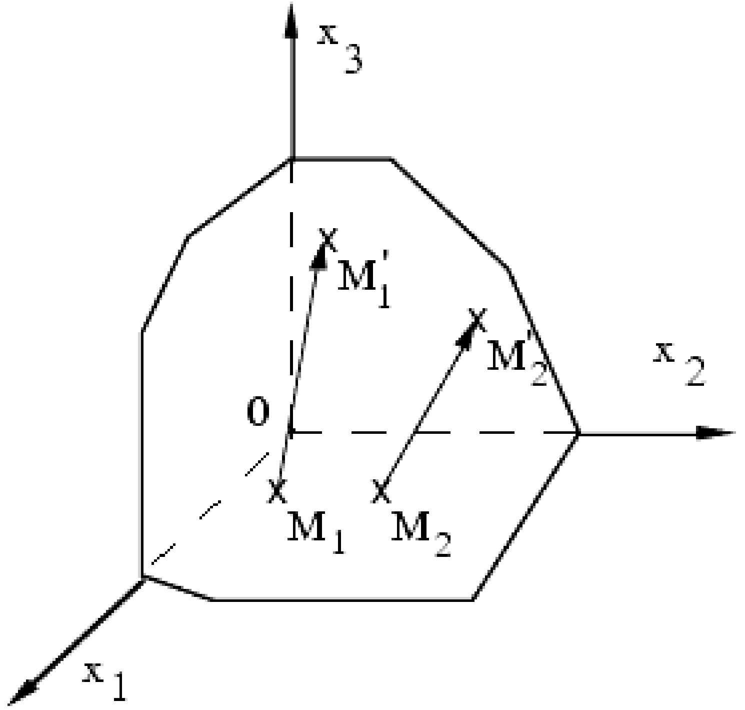
Strain tensors



$$dx'_i = dx_i + du_i$$

Landau-Lifshitz theory

$$dl = \sqrt{dx_1^2 + dx_2^2 + dx_3^2} \qquad dl' = \sqrt{dx'^2_1 + dx'^2_2 + dx'^2_3}$$

Before

After deformation

Distortion tensor β_{ik}

Displacement vector $\vec{u} = \vec{u}(x_1, x_2, x_3)$

$$\boxed{du_i = \frac{\partial u_i}{\partial x_k} dx_k = \beta_{ik} dx_k}$$

$$dl'^2 = (dx_i + du_i)^2$$

$$dl'^2 = dx_i^2 + 2dx_i du_i + du_i^2 = dl^2 + 2\frac{\partial u_i}{\partial x_k} dx_k dx_i + \frac{\partial u_i}{\partial x_k}\frac{\partial u_i}{\partial x_l} dx_k dx_l$$

$$dl'^2 = dl^2 + 2u_{ik} dx_k dx_i$$

Strain tensor u_{ik}

$$\boxed{u_{ik} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i} + \cancel{\frac{\partial u_l}{\partial x_k}\frac{\partial u_l}{\partial x_i}}\right) \simeq \frac{1}{2}\left(\frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i}\right)}$$

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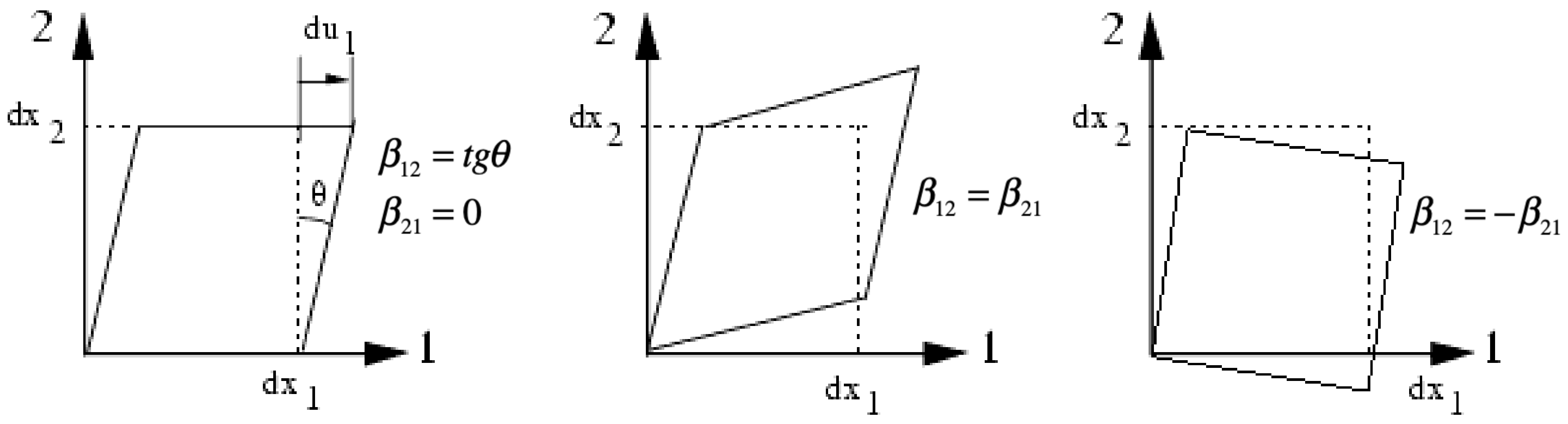
Physical significance of the strain tensor

$$dl'^2 = \left(\delta_{ik} + 2u_{ik}\right)dx_k dx_i = \left(1 + 2u^{(i)}\right)dx_i^2$$ since a basis exists where u_{ik} is diagonal

Kronecker's delta

in this basis $dx'_i = \sqrt{\left(1+2u^{(i)}\right)}dx_i \simeq \left(1+u^{(i)}\right)dx_i$

$$\frac{dV'}{dV} = \frac{dx'_1\,dx'_2\,dx'_3}{dx_1 dx_2 dx_3} = \prod_{i=1}^{3}\left(1+u^{(i)}\right) \simeq \left(1+u^{(1)}+u^{(2)}+u^{(3)}\right) = \left(1+tr(u)\right)$$



deformations rotations

$$\beta_{ik} = \frac{1}{2}\left(\beta_{ik}+\beta_{ki}\right) + \frac{1}{2}\left(\beta_{ik}-\beta_{ki}\right) = u_{ik} \quad + \quad \omega_{ik}$$

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Stress tensor

Volume forces

$$\int F_i dV$$

$$\boxed{u_{ik} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i}\right)}$$

We assume that forces can only act on surfaces and are transmitted to volume through the surfaces.

$$\int F_i dV = \int \frac{\partial \sigma_{ik}}{\partial x_k} dV = \oint \sigma_{ik} ds_k$$

Divergence theorem

equilibrium

$$\boxed{F_i = 0 \Rightarrow \frac{\partial \sigma_{ik}}{\partial x_k} = 0}$$

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Review of thermodynamics

1st principle

$$dE = \delta Q + \delta W$$

If reversible process

$$\delta Q = TdS = dQ$$

$$dE = TdS - PdV$$

If pressure=constant

$$dQ = TdS = dE + PdV = d(E + PV) = dH$$

The enthalpy (heat) is an exact differential

$$dH = TdS + VdP$$

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Review of thermodynamics

If temperature=constant

$$dW = dE - dQ = d(E - TS) = dF = dE - SdT - TdS$$

$$dF = -PdV - SdT \qquad dE = TdS - PdV$$

The Helmholtz free energy (work) is an exact differential

If temperature+pressure=constant

$$G = E - TS + PV = H - TS = F + PV$$

$$dG = -SdT + VdP = 0 \quad G \text{ minimum}$$

For N particles

$$dG = -SdT + VdP + \mu dN$$

$$G = \mu N \quad \text{is the chemical potential}$$

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Review of thermodynamics

How to use these thermodynamic functions?

Irreversible process

$$\frac{\delta Q}{dt} \leq T\frac{dS}{dt}$$

$$\frac{\delta Q}{dt} = \frac{dE + PdV}{dt} \leq T\frac{dS}{dt} \Rightarrow \frac{dE}{dt} - T\frac{dS}{dt} \leq \frac{-PdV}{dt}$$

If temperature&volume=constant

$$\frac{dE}{dt} - T\frac{dS}{dt} = \frac{d(E-TS)}{dt} = \frac{dF}{dt} \leq 0$$

F minimum

If temperature&pressure=constant

$$= \frac{d(E-TS+PV)}{dt} = \frac{dG}{dt} \leq \frac{VdP}{dt} = 0$$

G minimum

If V&S=constant

$$\frac{dE}{dt} = \frac{\delta Q}{dt} \leq T\frac{dS}{dt} = 0$$

E minimum

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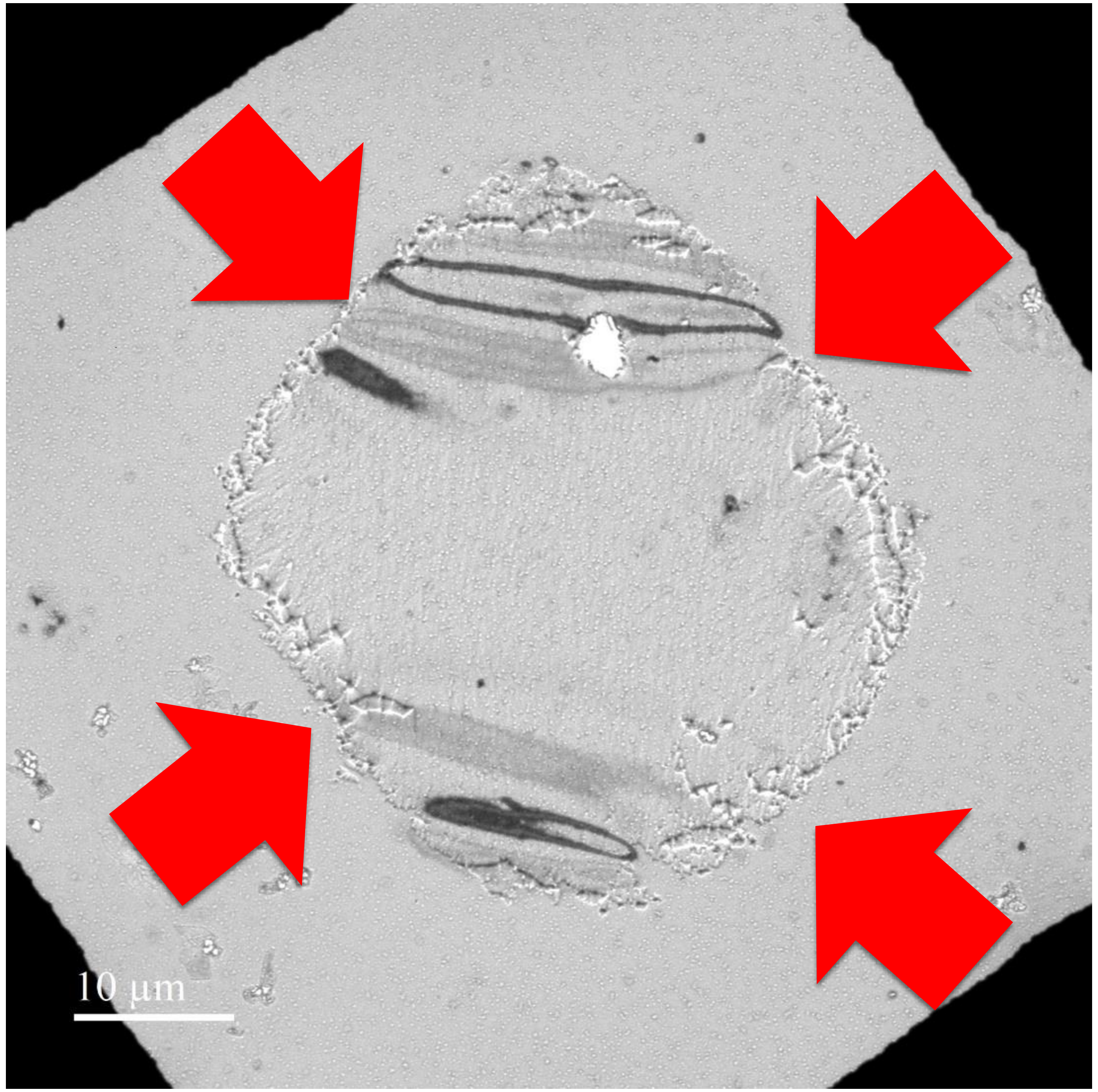
FM transition of FeRh within AFM phase induces elastic stresses



How do we express transformation stresses in FM transition?

Thermodynamics of deformation

Work of internal forces (! sign -)

$$\int \delta w_{\text{int}}\, dV = \int \frac{\partial \sigma_{ik}}{\partial x_k} \delta u_i dV$$

$$\int_V \delta w_{\text{int}}\, dV = \oint_\Sigma \sigma_{ik}\, \delta u_i\, ds_k - \int_V \sigma_{ik} \frac{d\delta u_i}{dx_k} dV$$

$$\int_V \delta w_{\text{int}}\, dV = -\int_V \sigma_{ik} \delta u_{ik} \cdot dV$$

$$\delta w_{\text{int}} = -\sigma_{ik} \delta u_{ik}$$

...per unit volume

Thermodynamics of deformation

Energy

$$de = \delta q - \delta w_{\text{int}} = Tds + \sigma_{ik} du_{ik}$$

Uniform compression

$$dE = TdS - pdu_{ll}V = TdS - p\frac{dV}{V}V = TdS - pdV$$

$$\boxed{df = -sdT + \sigma_{ik} du_{ik}}$$

$$\boxed{dh = Tds - u_{ik} d\sigma_{ik}}$$

$$\boxed{dg = -sdT - u_{ik} d\sigma_{ik}}$$

$$\sigma_{ik} = \left.\frac{\partial e}{\partial u_{ik}}\right)_S = \left.\frac{\partial f}{\partial u_{ik}}\right)_T$$

$$u_{ik} = -\left.\frac{\partial g}{\partial \sigma_{ik}}\right)_T = -\left.\frac{\partial g}{\partial \sigma_{ik}}\right)_S$$

Thermodynamics of deformation

The physical origin of the deformation

$$dF = -SdT - PdV + f_r dl \qquad f_r > 0$$

$$\boxed{f_r = \left.\frac{\partial F}{\partial l}\right)_{T,V} = \left.\frac{\partial E}{\partial l}\right)_{T,V} - T\left.\frac{\partial S}{\partial l}\right)_{T,V}} \qquad (1)$$

Internal energy variation

Entropy variation

Metals vs. Elastomers

F is an exact total differential

$$\frac{\partial}{\partial l}\left(\frac{\partial F}{\partial T}\right)_l = \frac{\partial}{\partial T}\left(\frac{\partial F}{\partial l}\right)_T \Rightarrow -\left.\frac{\partial S}{\partial l}\right)_{T,V} = \left.\frac{\partial f_r}{\partial T}\right)_{l,V} \qquad (2)$$

$$\boxed{f_r = \left.\frac{\partial E}{\partial l}\right)_{T,V} + T\left.\frac{\partial f_r}{\partial T}\right)_{l,V}} \qquad (1) + (2)$$

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Hooke's law

hypothesis | equilibrium:

Undeformed state

$$u_{ik} = 0 \Rightarrow \sigma_{ik} = 0$$

$$\sigma_{ik} = \left.\frac{\partial F}{\partial u_{ik}}\right)_T$$

F doesn't contain a linear term in u_{ik}, σ_{ik}

We search for invariants as coefficients of f, i.e, powers of u_{ik}

u_{ik} can be diagonalized, we can write the characteristic equation

$$Det\left(\bar{\bar{u}} - \lambda I\right) = 0 \Rightarrow \lambda^3 - Tr\left(\bar{\bar{u}}\right)\lambda^2 - C_2\lambda + Det\left(\bar{\bar{u}}\right) = 0$$

$$C_2 = u_{12}^2 + u_{13}^2 + u_{23}^2 - u_{11}u_{22} - u_{11}u_{33} - u_{22}u_{33}$$

but $\sum_{ik} u_{ik}^2 = \left[Tr\left(\bar{\bar{u}}\right)\right]^2 + 2C_2$ is also an invariant

$Tr\left(\bar{\bar{u}}\right) = u_{ii}$ first order invariant

$\left[Tr\left(\bar{\bar{u}}\right)\right]^2, C_2$ second order invariant

$Det\left(\bar{\bar{u}}\right)$ third order invariant

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Hooke's law

A possible form of free energy is:

$$f = f_0 + \frac{\lambda}{2}\left[Tr\left(\overline{\overline{u}}\right)\right]^2 + \mu \sum_{ik} u_{ik}^2$$

λ and μ are Lamé constants
λ ~ Young's modulus & ν
μ~ shear modulus

Search for a more physical form

$$u_{ik} = \underbrace{\left(u_{ik} - \frac{1}{3}\delta_{ik} \cdot Tr\left(\overline{\overline{u}}\right)\right)}_{\text{Pure shear}} + \underbrace{\frac{1}{3}\delta_{ik} \cdot Tr\left(\overline{\overline{u}}\right)}_{\text{hydrostatic pressure}}$$

$$\sum_{ik}\left(u_{ik} - \frac{1}{3}\delta_{ik} \cdot Tr\left(\overline{\overline{u}}\right)\right)^2$$ is also an invariant

$$\boxed{f = f_0 + \frac{K}{2}\left[Tr\left(\overline{\overline{u}}\right)\right]^2 + \mu \sum_{ik}\left(u_{ik} - \frac{1}{3}\delta_{ik} Tr\left(\overline{\overline{u}}\right)\right)^2}$$

with $K = \lambda + \frac{2}{3}\mu$

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Hooke's law

$$\sigma_{ik} = \left.\frac{\partial f}{\partial u_{ik}}\right)_T \Rightarrow \sigma_{ik} = 2\mu\left(u_{ik} - \frac{1}{3}\delta_{ik}\cdot Tr\left(\overline{\overline{u}}\right)\right) + \delta_{ik} K Tr\left(\overline{\overline{u}}\right)$$

Note that: $Tr\left(\overline{\overline{\sigma}}\right) = 3KTr\left(\overline{\overline{u}}\right)$

Hooke's law...depending on strains

$$u_{ik} = \frac{1}{2\mu}\left(\sigma_{ik} - \frac{1}{3}\delta_{ik}\cdot Tr\left(\overline{\overline{\sigma}}\right)\right) + \frac{1}{9K}\delta_{ik}\cdot Tr\left(\overline{\overline{\sigma}}\right)$$

Physical signification of μ and of K

Uniform compression: $\sigma_{ik} = -p\delta_{ik}$

$$Tr\left(\overline{\overline{u}}\right) = \frac{\Delta V}{V} = -\frac{p}{K} \qquad \frac{1}{K} = -\left(\frac{\partial V}{\partial P}\right)_T \frac{1}{V}$$

K is the compressibility modulus

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Hooke's law

Pure shear-stress $u_{12} = \frac{\theta}{2} \Rightarrow \sigma_{12} = \mu\theta$

μ is the shear modulus

Homogenous traction: $\sigma = \sigma_{33} \Rightarrow u_{33} = \frac{\sigma}{E} \Rightarrow E = \frac{9K\mu}{3K+\mu}$

$$u_{11} = u_{22} = -\nu\frac{\sigma}{E} \text{ with } \nu = \frac{1}{2}\frac{3K-2\mu}{3K+\mu} \Rightarrow -1 < \nu < \frac{1}{2}$$

New formulation of the Hooke's law:

$$\boxed{\sigma_{ik} = \frac{E}{1+\nu}\left(u_{ik} + \frac{\nu}{1-2\nu}\delta_{ik}\cdot Tr\left(\overline{\overline{u}}\right)\right)}$$

$$\boxed{u_{ik} = \frac{1}{E}\left((1+\nu)\sigma_{ik} - \nu\cdot\delta_{ik}\cdot Tr\left(\overline{\overline{\sigma}}\right)\right)}$$

Effect of temperature

$$\boxed{f = f_0(T) - K\alpha\left(T - T_0\right)Tr\left(\bar{\bar{u}}\right) + \frac{K}{2}\left[Tr\left(\bar{\bar{u}}\right)\right]^2 + \mu\sum_{ik}\left(u_{ik} - \frac{1}{3}\delta_{ik}Tr\left(\bar{\bar{u}}\right)\right)^2}$$

$$\sigma_{ik} = -K\alpha\left(T - T_0\right)\delta_{ik} + 2\mu\left(u_{ik} - \frac{1}{3}\delta_{ik}\cdot Tr\left(\bar{\bar{u}}\right)\right) + \delta_{ik}KTr\left(\bar{\bar{u}}\right)$$

$$\bar{\bar{\sigma}} = 0 \Rightarrow Tr\left(\bar{\bar{u}}\right) = \frac{\Delta V}{V} = \alpha\left(T - T_0\right)$$

Equilibrium equation of isotropic bodies $\quad u_{ik} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i}\right)$

$$\frac{\partial \sigma_{ik}}{\partial x_k} = 0 = \frac{E}{1+\nu}\left(\frac{\partial u_{ik}}{\partial x_k} + \frac{\nu}{1-2\nu}\frac{\partial Tr\left(\bar{\bar{u}}\right)}{\partial x_i}\right) = \frac{E}{2(1+\nu)}\frac{\partial^2 u_i}{\partial x_k^2} + \frac{E}{2(1+\nu)(1-2\nu)}\frac{\partial^2 u_l}{\partial x_l \partial x_i}$$

$$(1-2\nu)\Delta\vec{u} + \overrightarrow{grad}\left(div\left(\vec{u}\right)\right) = 0 \Rightarrow \Delta\Delta\vec{u} = 0$$

$\vec{u}$ is biharmonic

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Generalized Hooke's law

$$\sigma_{ij} = C_{ijkl} u_{kl}$$

energy $$W = \frac{1}{2}\sigma_{ij} u_{ij} = C_{ijkl} u_{kl} u_{ij}$$

Symmetry: 6 indices notation

$$11 \to 1,\ 22 \to 2,\ 33 \to 3,\ 23 \to 4,\ 31 \to 5,\ 12 \to 6$$

but $$u_4 = 2u_{23},\ u_5 = 2u_{31},\ u_6 = 2u_{12}$$

$$\begin{bmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{bmatrix} = \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{12} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{13} & C_{23} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{14} & C_{24} & C_{34} & C_{44} & C_{45} & C_{46} \\ C_{15} & C_{25} & C_{35} & C_{45} & C_{55} & C_{56} \\ C_{16} & C_{26} & C_{36} & C_{46} & C_{56} & C_{66} \end{bmatrix} \bullet \begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ u_6 \end{bmatrix}$$

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Generalized Hooke's law

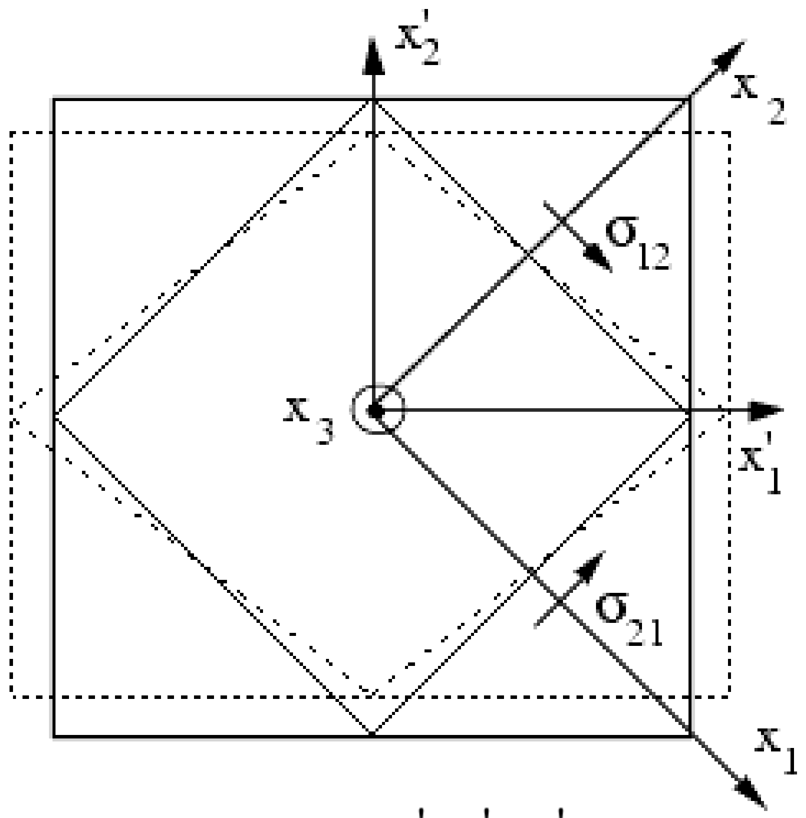
Crystalline system	C_{ij}	a_{ij}
triclinic	18	3
monoclinic	12	3
orthorhombic	9	3
tetrahedral	6	2
rhombohedral	6	2
hexagonal	5	2
cubic	3	1

Application to cubic crystals

$$C_{mn} = \begin{bmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{bmatrix}$$

$$\sigma_{11} = c_{11}u_{11} + c_{12}u_{22} + c_{12}u_{33}$$
$$\sigma_{22} = c_{12}u_{11} + c_{11}u_{22} + c_{12}u_{33}$$
$$\sigma_{33} = c_{12}u_{11} + c_{12}u_{22} + c_{11}u_{33}$$
$$\sigma_{23} = 2c_{44}u_{23}$$
$$\sigma_{31} = 2c_{44}u_{31}$$
$$\sigma_{12} = 2c_{44}u_{12}$$

Anisotropy coefficient



In $Ox_1^{'}x_2^{'}x_3^{'}$

$$\overline{\overline{\sigma}} = \begin{bmatrix} 0 & \sigma_{12} & 0 \\ \sigma_{12} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \qquad \overline{\overline{u}} = \begin{bmatrix} 0 & u_{12} & 0 \\ u_{12} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$\overline{\overline{\sigma}}' = \begin{bmatrix} \sigma_{11}^{'} & 0 & 0 \\ 0 & \sigma_{22}^{'} & 0 \\ 0 & 0 & 0 \end{bmatrix} \qquad \overline{\overline{u}}' = \begin{bmatrix} u_{11}^{'} & 0 & 0 \\ 0 & u_{22}^{'} & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

$$\sigma_{11}^{'} = \sigma_{12} \quad \sigma_{22}^{'} = -\sigma_{12} \qquad u_{11}^{'} = u_{12} \quad u_{22}^{'} = -u_{12}$$

Cubic $\quad \sigma_{11}^{'} = \sigma_{12} = 2C_{44}u_{12} \qquad \sigma_{11}^{'} = C_{11}u_{11}^{'} + C_{12}u_{22}^{'} = \left(C_{11} - C_{12}\right)u_{12}$

$2C_{44} = \left(C_{11} - C_{12}\right) \Rightarrow$ Anisotropy coefficient $\quad A = \dfrac{2C_{44}}{C_{11} - C_{12}}$

	Na	K	Fe	W	Al	Cu	Pb	C_{diam}	NaCl	KCl
A	7.5	5.7	2.4	1	1.2	3.2	4	1.6	0.7	0.36

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Inverse generalized Hooke law

$$u_{ij} = S_{ijkl}\sigma_{kl}$$

$$S_{ijkl} = S_{mn} \qquad m,\, n = 1,2,3$$

$$S_{ijkl} = \frac{1}{2}S_{mn} \qquad m \neq n = 4,5,6$$

$$S_{ijkl} = \frac{1}{4}S_{mn} \qquad m = n = 4,5,6$$

for instance

$$u_1 = S_{11}\sigma_1 + S_{12}\sigma_2 + S_{13}\sigma_3 + \frac{1}{2}\left(S_{14}\sigma_4 + S_{15}\sigma_5 + S_{16}\sigma_6\right)$$

Auxetic solid, $\nu<0$