

A Crystal Structure-Based Eigentransformation and Its Work-Conjugate Material Stress

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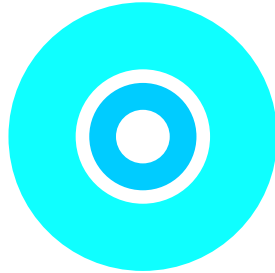
Eigenstrain and Eigentransformation

“Eigenstrain” is a generic name given by Toshio Mura to such nonelastic strains as thermal expansion, phase transformation, initial strains, plastic, misfit strains in his book *Micromechanics of Defects in Solids*.

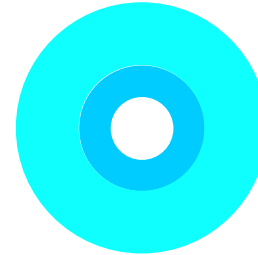
“Eigentransformation” is introduced as the nonlinear counterpart of eigenstrain in finite deformation.

Definition clear? Yes, if you know what you are doing.

Finite Shrink Fitting of Circular Rings



$$r_1^e(\mathbf{R}_{12}^{\text{SF}}) = r_2^e(\mathbf{R}_{21}^{\text{SF}})$$



SF Configuration in \mathbf{R}^{SF}

Ring 1: $R_{11}^{\text{SF}} < R^{\text{SF}} < R_{12}^{\text{SF}}$

Ring 2: $R_{21}^{\text{SF}} < R^{\text{SF}} < R_{22}^{\text{SF}}$

Spatial Configuration in r

$$r = r_1^e(\mathbf{R}^{\text{SF}})$$

$$r = r_2^e(\mathbf{R}^{\text{SF}})$$

The stress-free (SF) configuration consists of two mismatched rings but the final configuration after elastic (e) fitting is a single composite ring without a visible geometric discontinuity. Problem solved.

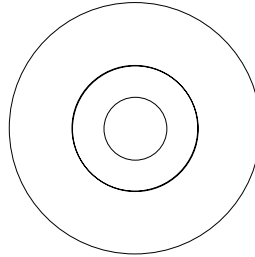
Where and what are the eigentransformations? What can they contribute to the understanding of material or configurational stresses?

Eigentransformations in Shrink Fitting

Referential in R

$$R_{11} < R < R_{12} = R_{21}$$

$$R_{21} < R < R_{22}$$

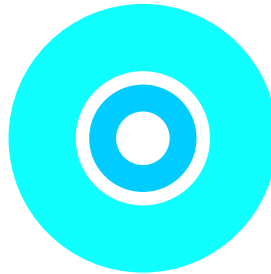


The disjointed SF rings may be mapped from a single contiguous annular referential configuration via eigenstretchratios Λ_1^*, Λ_2^* :

Stress – Free in R^{SF}

$$R_{11}^{SF} < R^{SF} < R_{12}^{SF} \neq R_{21}^{SF}$$

$$R_{21}^{SF} < R^{SF} < R_{22}^{SF}$$



$$R^{SF} = \Lambda_1^* R \quad (R_{11} < R < R_{12})$$

$$R^{SF} = \Lambda_2^* R \quad (R_{21} < R < R_{22})$$

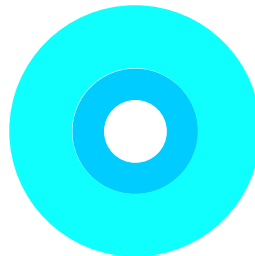
Since $R_{12} = R_{21}$

$$\Lambda_1^* / \Lambda_2^* = R_{12}^{SF} / R_{21}^{SF}$$

Spatial in r

$$r_{11} < r < r_{12} = r_{21}$$

$$r_{21} < r < r_{22}$$



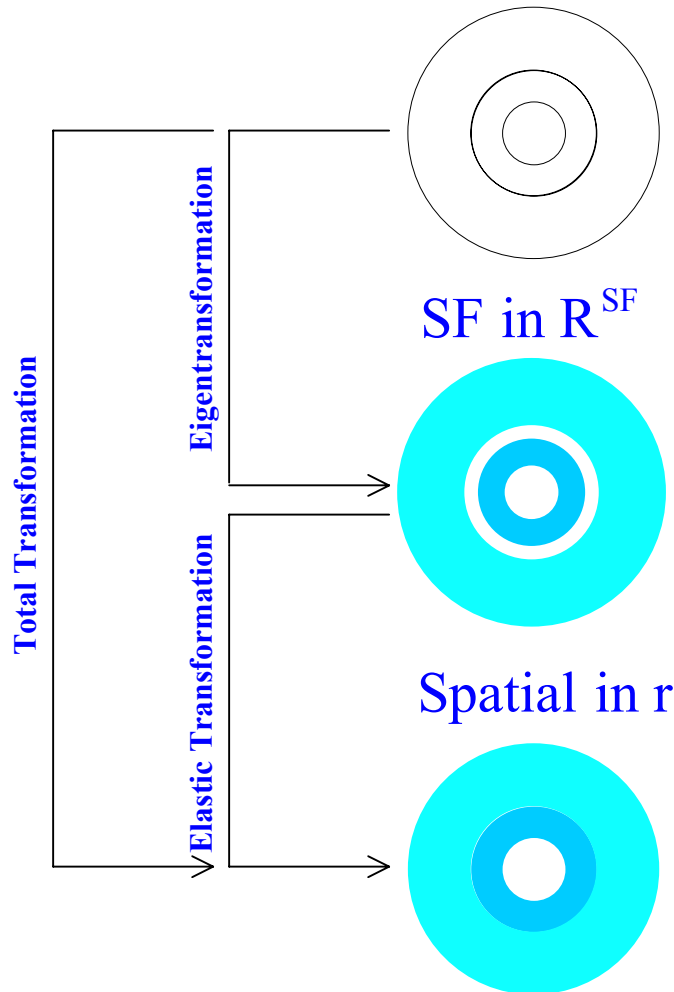
Coherence in terms of material length parameters ℓ_1, ℓ_2 :

$$R_{12}^{SF} / R_{21}^{SF} = \ell_1 / \ell_2$$

**Eigentransformations depend on the choice of referential configuration.
Requirement on coherent interface.**

The Shrink Fitting Experience

Referential in R



Choose a contiguous referential configuration—a 3-D grid work with empty cells.

Fill the cells with component elements and they will combine to assume their natural stress-free cell shapes. These cells, in general, cannot be fitted together to form a stress-free body.

Since the spatial configuration is required to be a contiguous body, an elastic transformation must be superimposed on each SF cell.

An N-Component system

Partial Molar Density (Molar Concentration) for Component m

Per Unit Referential Volume in \mathbf{X} : C_m $C = \sum C_m$

Per Unit Spatial Volume in \mathbf{x} : c_m $c = \sum c_m$

Per Unit Stress-Free Volume : C_m^{SF} $C^{\text{SF}} = \sum C_m^{\text{SF}}$

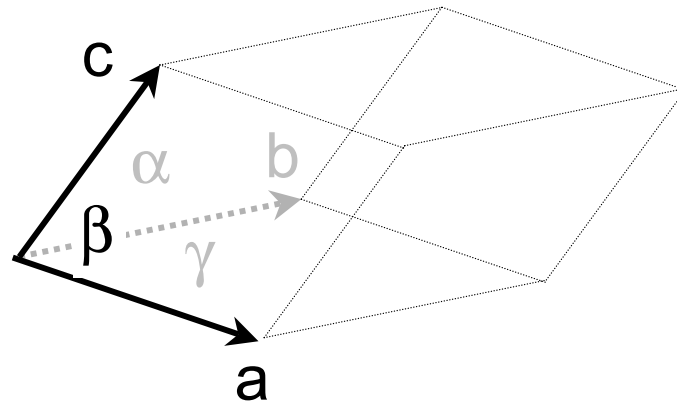
Mole Fraction (Composition): $x_m = C_m/C = c_m/c = C_m^{\text{SF}}/C^{\text{SF}}$

Jacobians of Transformation

$$\left\{ \begin{array}{l} J = dv/dV = C/c = C_m/c_m \\ J^e = dv/dV^{\text{SF}} = C^{\text{SF}}/c = C_m^{\text{SF}}/c_m \\ J^* = dV^{\text{SF}}/dV = C/C^{\text{SF}} = C_m/C_m^{\text{SF}} \end{array} \right.$$

An N-Component Alloy Crystal

A unit cell of edge lengths (a, b, c) and interaxial angles (α, β, γ)



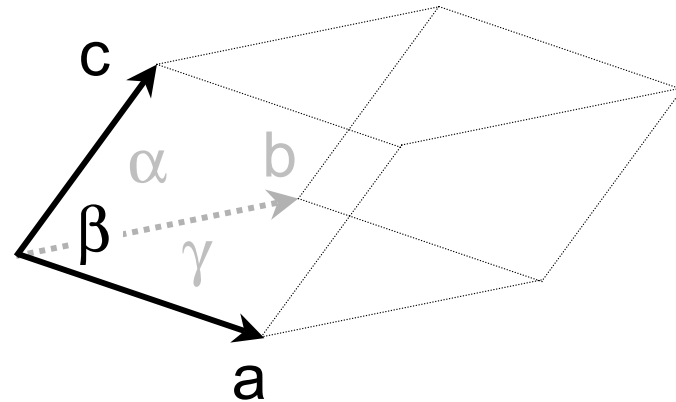
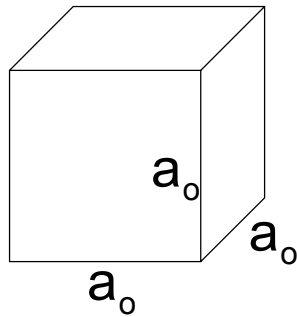
The six lattice parameters, or lattice constants $p \equiv (a, b, c; \alpha, \beta, \gamma)$, for a unit cell are, in general, functions of the composition, i.e.

$$p = p(\underline{x}) \equiv p(x_1, \dots, x_{N-1})$$

The total number of atoms per cell is N_{cell} .

A Referential Simple Cubic Cell

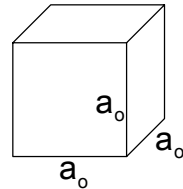
A simple cubic cell of lattice constants $p \equiv (a, b, c; \alpha, \beta, \gamma)$
 $= (a_0, a_0, a_0; 90^\circ, 90^\circ, 90^\circ)$ is used to define a referential configuration



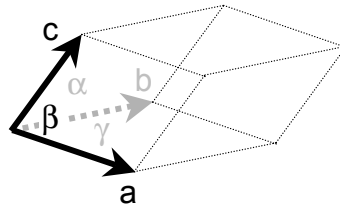
The mapping from the simple cubic cell $p = (a_0, a_0, a_0; 90^\circ, 90^\circ, 90^\circ)$ to the alloy crystal cell $p(\underline{x}) \equiv (a, b, c; \alpha, \beta, \gamma)(\underline{x})$ gives the desired eigentransformation \mathbf{F}^* , which, together with $p(\underline{x})$, varies as a function of time via its dependence on the composition \underline{x} .

A collection of Nonuniform SF Cells

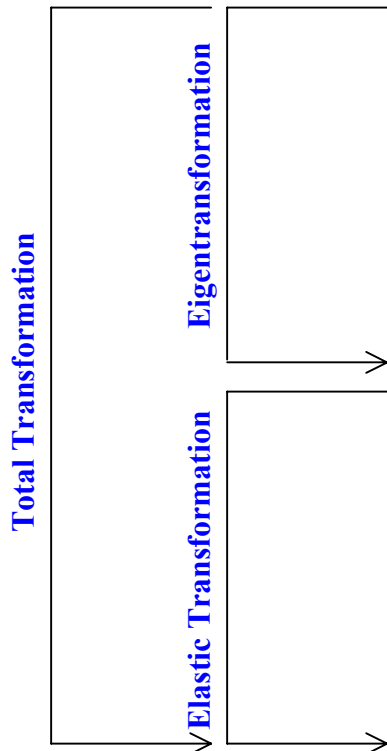
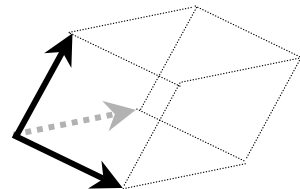
Referential in \mathbf{X}



SF in \mathbf{X}^{SF}



Spatial in \mathbf{x}



Fill each cell with N_{cell} atoms in accordance with the non-uniform composition \underline{x} .

The N_{cell} atoms will combine into a SF crystal cell via eigentransformation \mathbf{F}^* .

An elastic transformation \mathbf{F}^e is then developed in response to the nonuniform \mathbf{F}^* .

The total transformation is just $\mathbf{F} = \mathbf{F}^e \mathbf{F}^*$.

The Helmholtz Free Energy

$$\begin{array}{ccccccc} & \text{Helmholtz per unit} & \text{Molar} & \text{Molar} & \text{Piola . Deformation} \\ & \text{referential volume} & \text{Helmholtz} & \text{Gibbs} & \text{Gradient} \\ \text{---} & \text{---} & \text{---} & \text{---} & \text{---} \\ \underline{A}(\mathbf{F}, T, C_m) = C \underline{A}(\mathbf{F}, T, \mathbf{x}) = C \underline{G}(\mathbf{S}, T, \mathbf{x}) + \mathbf{S} \cdot \mathbf{F} & \text{and} & \mathbf{F} = \mathbf{F}^e \mathbf{F}^* \end{array}$$

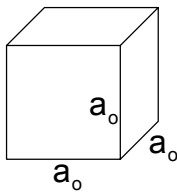
$\underline{A}(\mathbf{1}, T_o, \mathbf{x}_o) = 0$ as a reference

$\underline{A}(\mathbf{F}^*, T, \mathbf{x}) = \underline{G}^{\text{SF}}(T, \mathbf{x}) \equiv \underline{G}(\mathbf{S}, T, \mathbf{x})|_{\mathbf{S}=0}$, \mathbf{F}^* stress - free eigentransformation

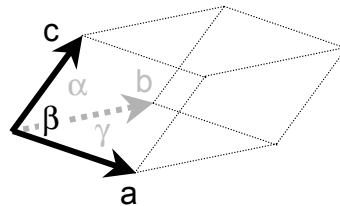
$\underline{A}(\mathbf{F}, T, \mathbf{x}) = \underline{A}(\mathbf{F}^e \mathbf{F}^*, T, \mathbf{x}) = \underline{A}(\mathbf{F}^*, T, \mathbf{x}) + [\underline{A}(\mathbf{F}^e \mathbf{F}^*, T, \mathbf{x}) - \underline{A}(\mathbf{F}^*, T, \mathbf{x})]$

Define: $\underline{W}^{\text{SF}}(\mathbf{F}^e, T) \equiv \underline{A}(\mathbf{F}^e \mathbf{F}^*, T, \mathbf{x}) - \underline{A}(\mathbf{F}^*, T, \mathbf{x})$, $\underline{W}^{\text{SF}}(\mathbf{1}, T) = 0$

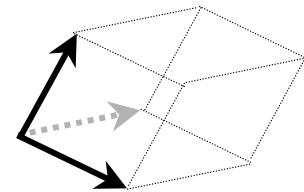
The dependence of elasticity on composition is usually insignificant.



Referential in \mathbf{X}



SF in \mathbf{X}^{SF}



Spatial in \mathbf{x}

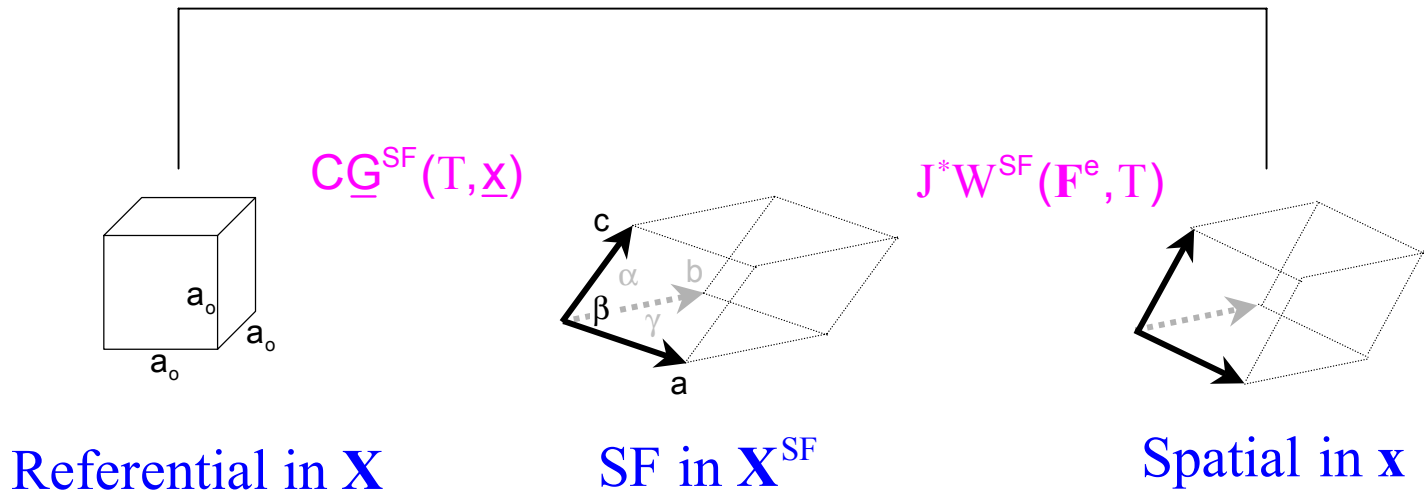
The Helmholtz Free Energy--Conclusion

$$A(\mathbf{F}, T, C_m) = CA(\underline{\mathbf{F}}^e \mathbf{F}^*, T, \underline{\mathbf{x}}) = C [\underline{A}(\mathbf{F}^*, T, \underline{\mathbf{x}}) + \underline{W}^{\text{SF}}(\mathbf{F}^e, T)], \text{ or}$$

$$A = C \underline{G}(0, T, \underline{\mathbf{x}}) + \frac{C}{C^{\text{SF}}} [C^{\text{SF}} \underline{W}^{\text{SF}}(\mathbf{F}^e, T)] = \underline{C} \underline{G}^{\text{SF}}(T, \underline{\mathbf{x}}) + J^* \underline{W}^{\text{SF}}(\mathbf{F}^e, T)$$

Stress-free molar Gibbs
Stress-free strain energy

$$A = \underline{C} \underline{G}^{\text{SF}}(T, \underline{\mathbf{x}}) + J^* \underline{W}^{\text{SF}}(\mathbf{F}^e, T)$$



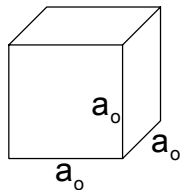
Piola Stresses

HELMHOLTZ ENERGY

$$A(\mathbf{F}, T, C_m) = \underbrace{C\bar{G}^{\text{SF}}(T, \underline{\mathbf{x}})}_{\text{Stress-free molar Gibbs}} + \underbrace{J^* W^{\text{SF}}(\mathbf{F}^e, T)}_{\text{strain energy density per unit stress-free volume}}$$

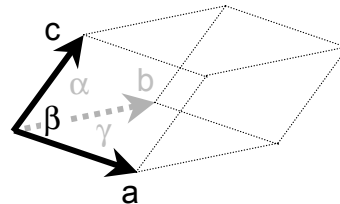
W strain energy density per unit referential volume

Piola Stress: $\mathbf{S} = \frac{\partial A}{\partial \mathbf{F}} = \frac{\partial W}{\partial \mathbf{F}} = J^* \mathbf{S}^e (\mathbf{f}^*)^T$ where $\mathbf{S}^e \equiv \frac{\partial W^{\text{SF}}}{\partial \mathbf{F}^e}$, $\mathbf{f}^* = (\mathbf{F}^*)^{-1}$



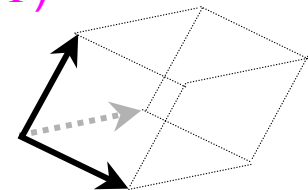
Referential in \mathbf{X}

$$C\bar{G}^{\text{SF}}(T, \underline{\mathbf{x}})$$



SF in \mathbf{X}^{SF}

$$J^* W^{\text{SF}}(\mathbf{F}^e, T)$$



Spatial in \mathbf{x}

Chemical Potential and Eshelby Stress

HELMHOLTZ FREE ENERGY

$$A(\mathbf{F}, T, \mathbf{C}_m) = C \underline{G}^{\text{SF}}(T, \underline{\mathbf{x}}) + J^* W^{\text{SF}}(\mathbf{F}^e, T)$$

CHEMICAL POTENTIAL

$$\mu_m = \frac{\partial A}{\partial \mathbf{C}_m} = \frac{\partial}{\partial \mathbf{C}_m} C \underline{G}^{\text{SF}}(T, \underline{\mathbf{x}}) + \frac{\partial}{\partial \mathbf{C}_m} J^* W^{\text{SF}}(\mathbf{F}^e, T), \quad \mathbf{F}^e = \mathbf{F}(\mathbf{F}^*)^{-1}$$

$$\mu_m = \bar{G}^{\text{SF}}(T, \underline{\mathbf{x}}) + J^* \mathbf{C}^e \cdot \left[\frac{\partial \mathbf{F}^*}{\partial \mathbf{C}_m} (\mathbf{f}^*)^T \right] \quad \text{or} \quad \mathbf{C} \cdot \left[\mathbf{f}^* \frac{\partial \mathbf{F}^*}{\partial \mathbf{C}_m} \right]$$

PARTIAL MOLAR GIBBS ENERGY

$$\bar{G}^{\text{SF}}(T, \underline{\mathbf{x}}) = \frac{\partial}{\partial \mathbf{C}_m} C \underline{G}^{\text{SF}}(T, \underline{\mathbf{x}})$$

GENERALIZED MATERIAL (or ESHELBY or CONFIGURATIONAL) STRESS

$$\mathbf{C}^e = W^{\text{SF}} \mathbf{1} - (\mathbf{F}^e)^T \mathbf{S}^e : \text{Relative to Stress-Free Configuration}$$

$$\mathbf{C} = J^* W^{\text{SF}} \mathbf{1} - \mathbf{F}^T \mathbf{S} : \text{Relative to Referential Configuration}$$

A Summary via A Binary System

$$\mathbf{X} \quad \begin{array}{c} \xleftarrow{\mathbf{F} \text{ and } \mathbf{J}} \\ \xrightarrow{\mathbf{f} \text{ and } \mathbf{j}} \end{array} \quad \mathbf{x}$$

Concentrations 1 [mol/m ³]	$C_1(\mathbf{X}, t) = Jc_1$	$jC_1 = c_1(\mathbf{x}, t)$
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Concentrations 2 [mol/m ³]	$C_2(\mathbf{X}, t) = Jc_2$	$jC_2 = c_2(\mathbf{x}, t)$
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Total	$C = Jc(\mathbf{x}, t)$	$jC = c(\mathbf{x}, t)$
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Mass Flux 1 [mol/m ² s]	$\mathbf{J}_1(\mathbf{X}, t) = C_1\mathbf{V}_1$	$c_1\mathbf{v}_1 = \mathbf{j}_1(\mathbf{x}, t)$
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Mass Flux 2 [mol/m ² s]	$\mathbf{J}_2(\mathbf{X}, t) = C_2\mathbf{V}_2$	$c_2\mathbf{v}_2 = \mathbf{j}_2(\mathbf{x}, t)$
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Balance Law	$\partial C_1 / \partial t = -\text{Div } \mathbf{J}_1$	$c\dot{x}_1 = -\text{div } \mathbf{j}_1$
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Balance Law	$\partial C_2 / \partial t = -\text{Div } \mathbf{J}_2$	$c\dot{x}_2 = -\text{div } \mathbf{j}_2$
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Mole Fractions	$x_1 + x_2 = 1,$	$\mathbf{J}_1 + \mathbf{J}_2 = 0$
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A Binary System -- Thermodynamics

Referential Representation

Energy Balance

$$\dot{U} = \dot{Q}_h + \dot{\mathbf{x}}_{,I} \cdot \mathbf{T}_I$$

Second Law

$$T\dot{S} - \dot{Q}_h - \frac{1}{T} \mathbf{J}_h \cdot \text{Grad } T + \mu_1 \dot{C}_1 - T \mathbf{J}_1 \cdot \text{Grad } \frac{\mu_1}{T} + \mu_2 \dot{C}_2 - T \mathbf{J}_2 \cdot \text{Grad } \frac{\mu_2}{T} \geq 0$$

Combining and in terms of Helmholtz Energy : $A = U - TS$

Dissipation Inequality

$$-\left[\dot{A} + S\dot{T} - \mathbf{S} \cdot \dot{\mathbf{F}} - \mu_1 \dot{C}_1 - \mu_2 \dot{C}_2\right] - \frac{1}{T} [\mathbf{J}_h - \mu_1 \mathbf{J}_1 - \mu_2 \mathbf{J}_2] \cdot \text{Grad } T \\ - \mathbf{J}_2 \cdot \text{Grad } \mu_2 - \mathbf{J}_1 \cdot \text{Grad } \mu_1 \geq 0$$

A Binary System -- Dissipation Inequality

$$-\mathbf{J}_h \cdot \frac{1}{T} \text{Grad } T - \mathbf{J}_1 \cdot \left[\text{Grad } \mu_1 - \frac{\mu_1}{T} \text{Grad } T \right] \\ - \mathbf{J}_2 \cdot \left[\text{Grad } \bar{\mu}_2 - \frac{\mu_2}{T} \text{Grad } T \right] \geq 0$$

Using $\mathbf{J}_1 + \mathbf{J}_2 = 0$ and for isothermal cases

$$-\mathbf{J}_1 \cdot \text{Grad } [\mu_1 - \mu_2] \geq 0$$

PHENOMENOLOGICAL CONSTANT D

$$\mathbf{J}_1 = -\frac{DC_1}{RT} \nabla [\mu_1 - \mu_2] \quad \partial C_1 / \partial t = -\text{Div } \mathbf{J}_1$$

Diffusion Coefficient D [m²/s], Temperature T [K]

Molar Boltzmann constant R [J/mol K]

A Binary System – Chemical Potential

$$\mathbf{J}_1 = -\frac{DC_1}{RT} \nabla [\mu_1 - \mu_2] \quad \partial C_1 / \partial t = -\text{Div } \mathbf{J}_1$$

chemical potential

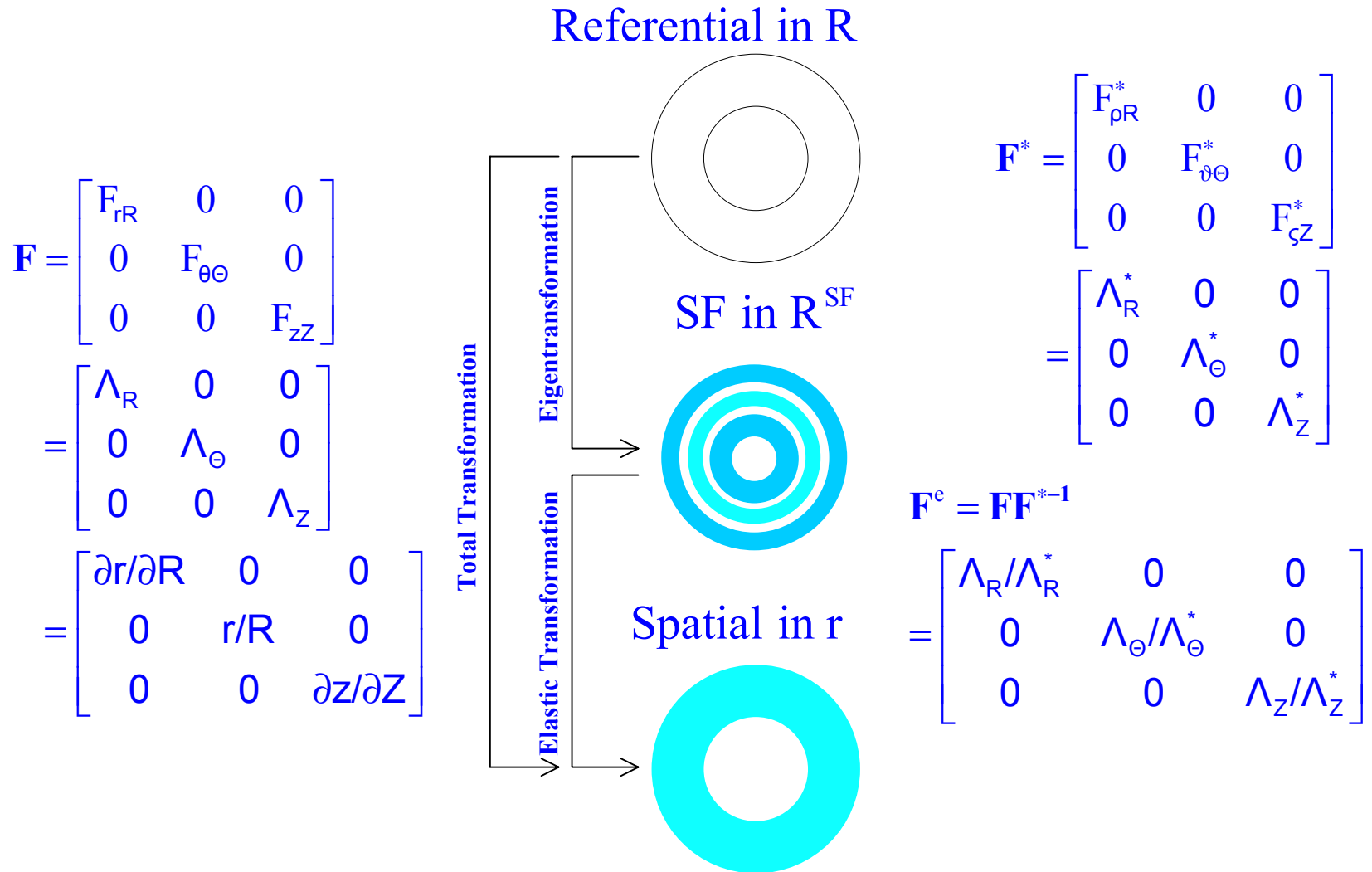
Diffusion Coefficient D [m²/s], Molar Boltzmann constant R [J/mol K]

In terms of stress-free molar Gibbs Energy $\underline{G}^{\text{SF}}(T, \mathbf{x}_1)$, strain energy density $W^{\text{SF}}(\mathbf{F}^e, T)$ and eigentransformation $\mathbf{F}^*(\mathbf{x}_1)$, where $\mathbf{x}_1 = \mathbf{C}_1/\mathbf{C}$, $\mathbf{x}_2 = \mathbf{1} - \mathbf{x}_1$, $\mathbf{C} = \mathbf{C}_1 + \mathbf{C}_2$ and $\mathbf{F}^e = \mathbf{F}(\mathbf{F}^*)^{-1}$.

$$\mu_1 - \mu_2 = \frac{\partial \underline{G}^{\text{SF}}}{\partial \mathbf{x}_1} + \mathbf{J}^* \mathbf{C}^e \cdot \left[\frac{1}{\mathbf{C}} \frac{\partial \mathbf{F}^*}{\partial \mathbf{x}_1} (\mathbf{f}^*)^T \right] \quad \text{or} \quad \mathbf{C} \cdot \left[\mathbf{f}^* \frac{1}{\mathbf{C}} \frac{\partial \mathbf{F}^*}{\partial \mathbf{x}_1} \right]$$

$$\mathbf{C}^e = W^{\text{SF}} \mathbf{1} - (\mathbf{F}^e)^T \mathbf{S}^e, \quad \mathbf{C} = \mathbf{J}^* W^{\text{SF}} \mathbf{1} - \mathbf{F}^T \mathbf{S}$$

Example – Cylindrically Orthotropic Cylinder

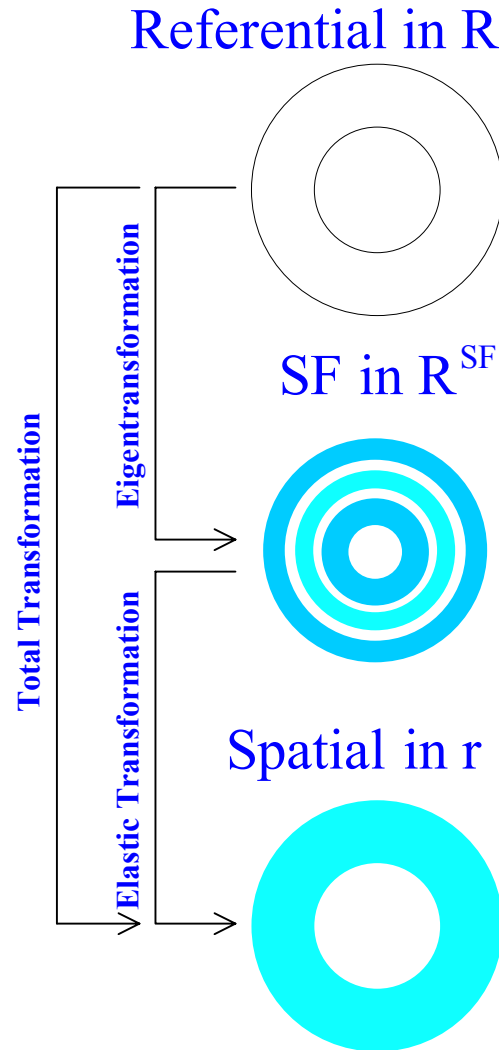


Cylindrically Orthotropic Cylinder -- Stresses

$$P_R = \frac{\partial A}{\partial \Lambda_R} = \frac{\partial W}{\partial \Lambda_R} = \frac{J^*}{\Lambda_R^*} P_R^e$$

$$P_\Theta = \frac{\partial A}{\partial \Lambda_\Theta} = \frac{\partial W}{\partial \Lambda_\Theta} = \frac{J^*}{\Lambda_\Theta^*} P_\Theta^e$$

$$P_Z = \frac{\partial A}{\partial \Lambda_Z} = \frac{\partial W}{\partial \Lambda_Z} = \frac{J^*}{\Lambda_Z^*} P_Z^e$$



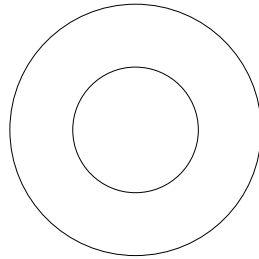
$$P_R^e = \frac{\partial W^{SF}}{\partial \Lambda_R^e}$$

$$P_\Theta^e = \frac{\partial W^{SF}}{\partial \Lambda_\Theta^e}$$

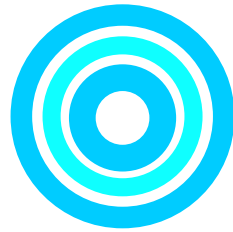
$$P_Z^e = \frac{\partial W^{SF}}{\partial \Lambda_Z^e}$$

Cylindrically Orthotropic Cylinder Chemical Potential

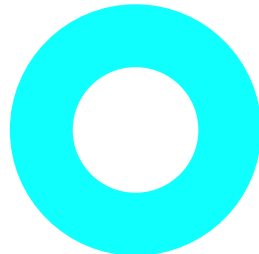
Referential in R



SF in R^{SF}



Spatial in r



Total Transformation

Eigentransformation

Elastic Transformation

$$\mu_a = \mu_a^{SF} + \left[\Sigma_R \left(\frac{1}{\Lambda_R^*} \frac{\partial \Lambda_R^*}{\partial C_a} \right) + \Sigma_\Theta \left(\frac{1}{\Lambda_\Theta^*} \frac{\partial \Lambda_\Theta^*}{\partial C_a} \right) + \Sigma_Z \left(\frac{1}{\Lambda_Z^*} \frac{\partial \Lambda_Z^*}{\partial C_a} \right) \right]$$

$$\mu_1^{SF} = \bar{G}_1^{SF}(T, x_1) = \frac{\partial}{\partial C_1} [CG^{SF}(T, x_1)]$$

$$\Sigma_R = W - P_R \Lambda_R = J^* \Sigma_R^{SF}, \quad \Sigma_R^{SF} = W^{SF} - P_R^e \Lambda_R^e$$

$$\Sigma_\Theta = W - P_\Theta \Lambda_\Theta = J^* \Sigma_\Theta^{SF}, \quad \Sigma_\Theta^{SF} = W^{SF} - P_\Theta^e \Lambda_\Theta^e$$

$$\Sigma_Z = W - P_Z \Lambda_Z = J^* \Sigma_Z^{SF}, \quad \Sigma_Z^{SF} = W^{SF} - P_Z^e \Lambda_Z^e$$

Σ : Principal configurational stresses

Conclusion

[1] It is known that the shape and volume of the unit cells of a crystal may be affected by its alloy composition. An eigentransformation, relative to an arbitrarily chosen reference, is introduced to measure this "material difference."

[2] The use of a 3-D simple-cubic-lattice grid work as a common reference is found to be most convenient, especially in the treatment of bicrystal interfaces.

[3] A generalized material (or Eshelby or configurational) stress is shown to be work conjugate to the eigentransformation.

[4] The known phenomena of finite elastic deformation and atomic diffusion are seamlessly merged into a unified theory.

[5] Results pertinent to a cylindrically orthotropic elastic cylinder are presented as an example.

Thank You!