Computing Bifurcation & Stability Properties of Crystals

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Outline

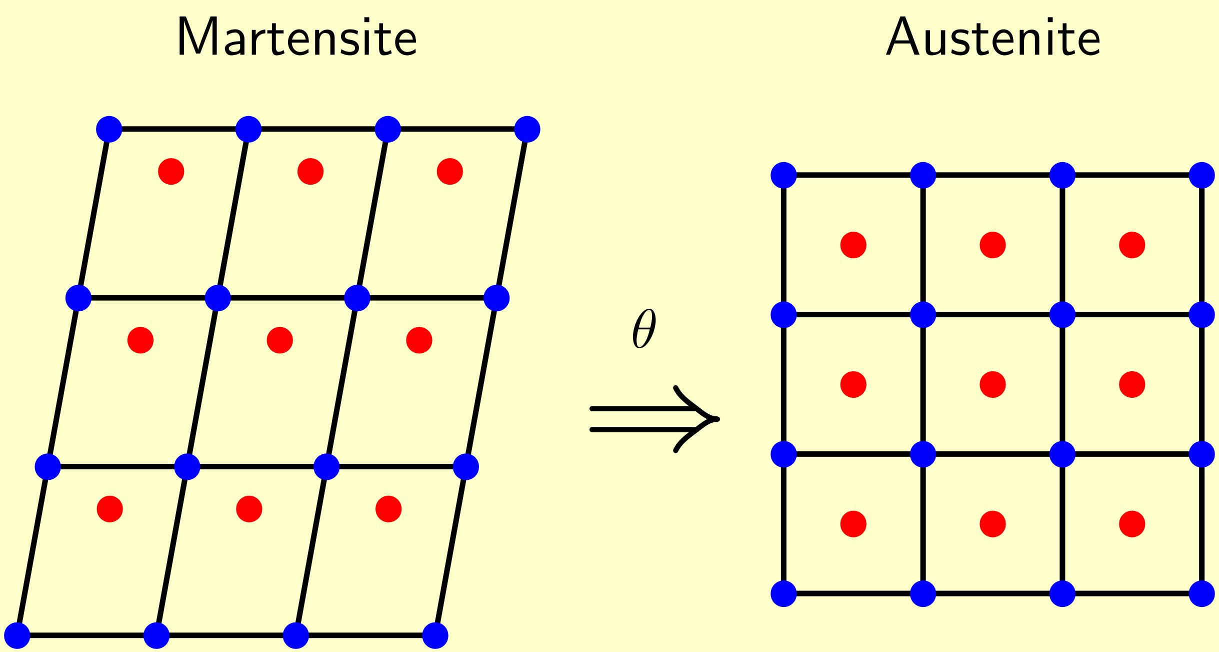
- Introduction & motivation
  - Active materials & Martensitic transformations (MT's)
  - Shape Memory Alloys (SMA's)
- Atomistic modeling of MT's
  - Temperature-dependent atomic potentials
  - Bifurcation & stability investigation of stress-free phases
  - Hysteretic proper MT between cubic $B2$ and orthorhombic $B19$ phases
- Computational challenges
  - Crystal stability
  - Equilibrium path following
  - Behavior near bifurcation points
- Summary & conclusions

Active Materials

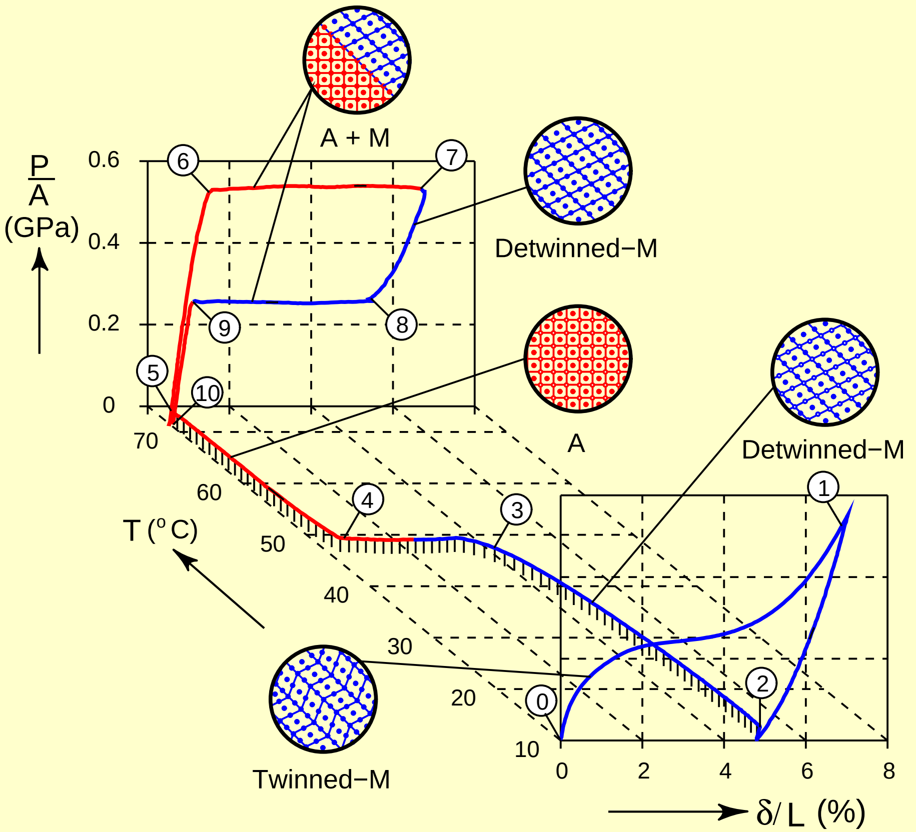
- Multi-physics coupling — Crystal structure changes

Magnetostrictive Materials	Magnetic Field	$\leftrightarrow$	Mechanical
Ferroelectric Materials	Electric Field	$\leftrightarrow$	Mechanical
Shape Memory Alloys	Temperature	$\leftrightarrow$	Mechanical

Martensitic Transformations
Materials on the cusp of an instability



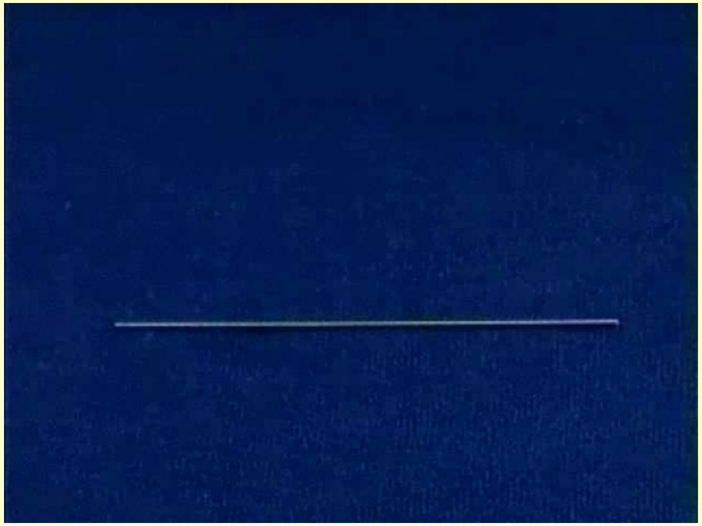
Shape Memory Alloys (SMAs)



Tensile behavior of NiTi

(exhibiting the shape memory effect and pseudo−elasticity)

(J. Shaw 1997)



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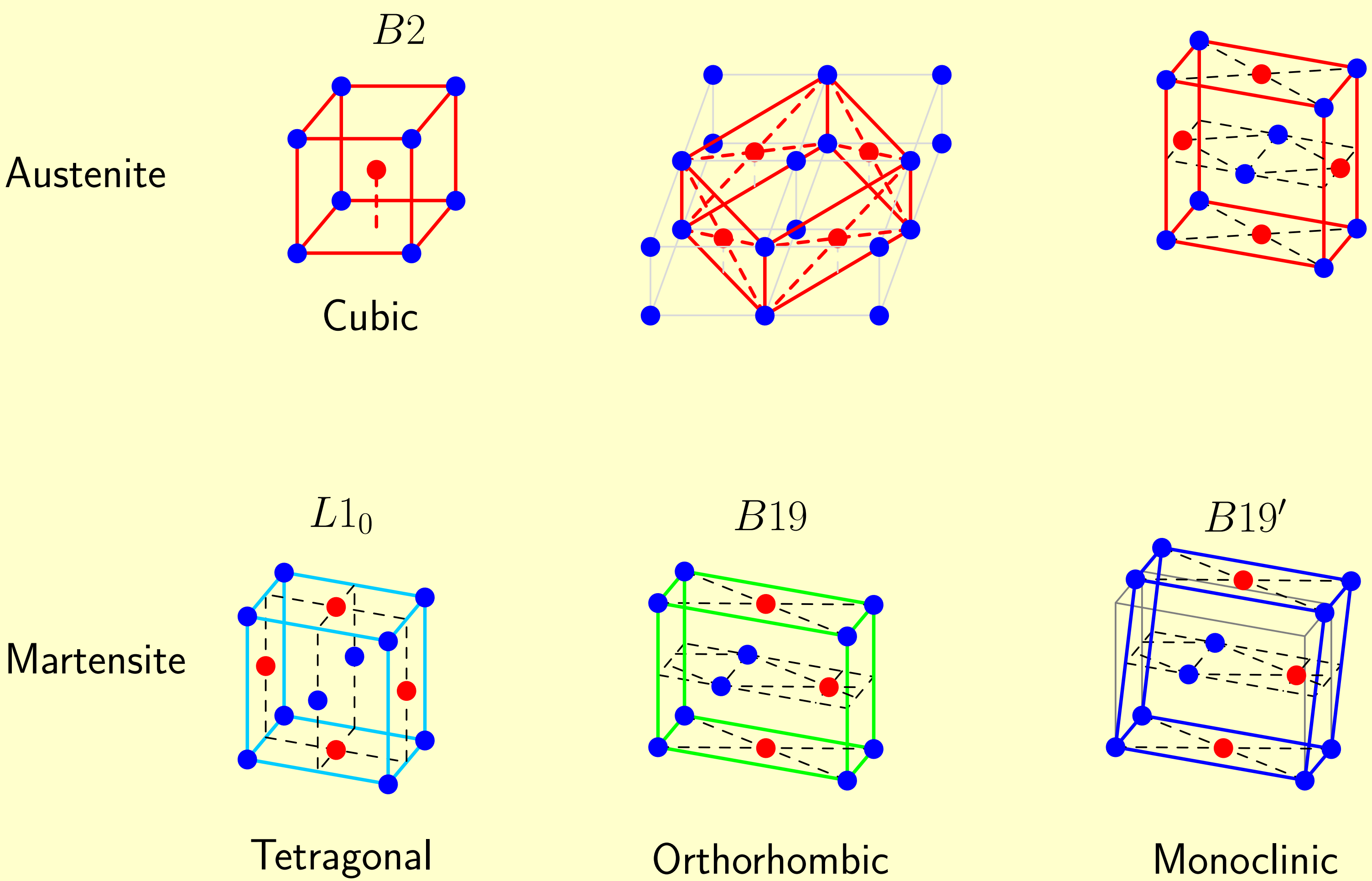
www.mrsec.wisc.edu/nano

The Crystal Structures of SMAs

- Prevalent austenite and martensite crystals in shape memory alloys



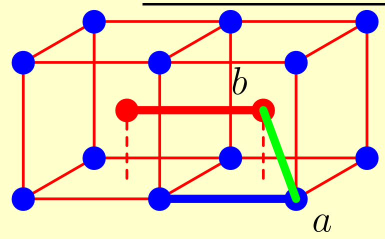
Objective: Develop an atomic model to capture *proper* martensitic transformations such as those found in shape memory alloys

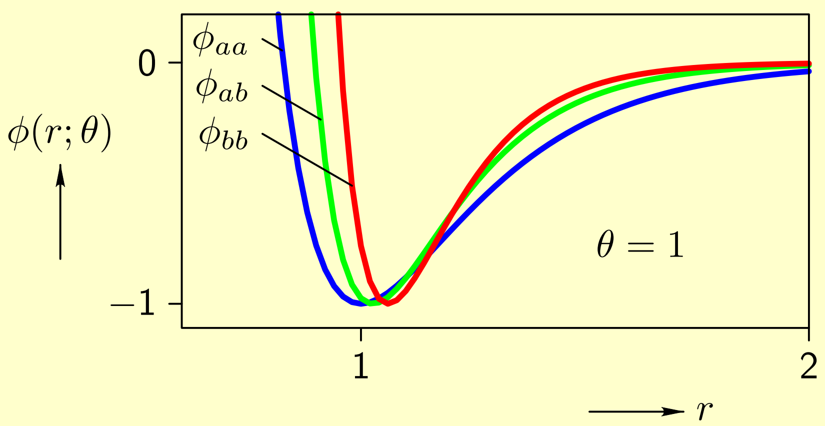
Pair-Potential Model

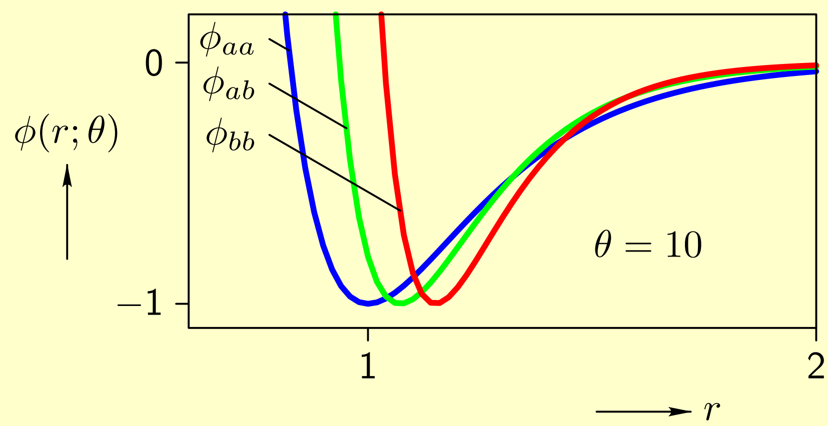
$$\phi(r;\theta) = A\left\{\exp\left[-2B\left(\frac{r}{\hat{r}(\theta)}-1\right)\right] - 2\exp\left[-B\left(\frac{r}{\hat{r}(\theta)}-1\right)\right]\right\}$$

$$\hat{r}(\theta) = r_0 + r_\theta\,(\theta - 1)$$

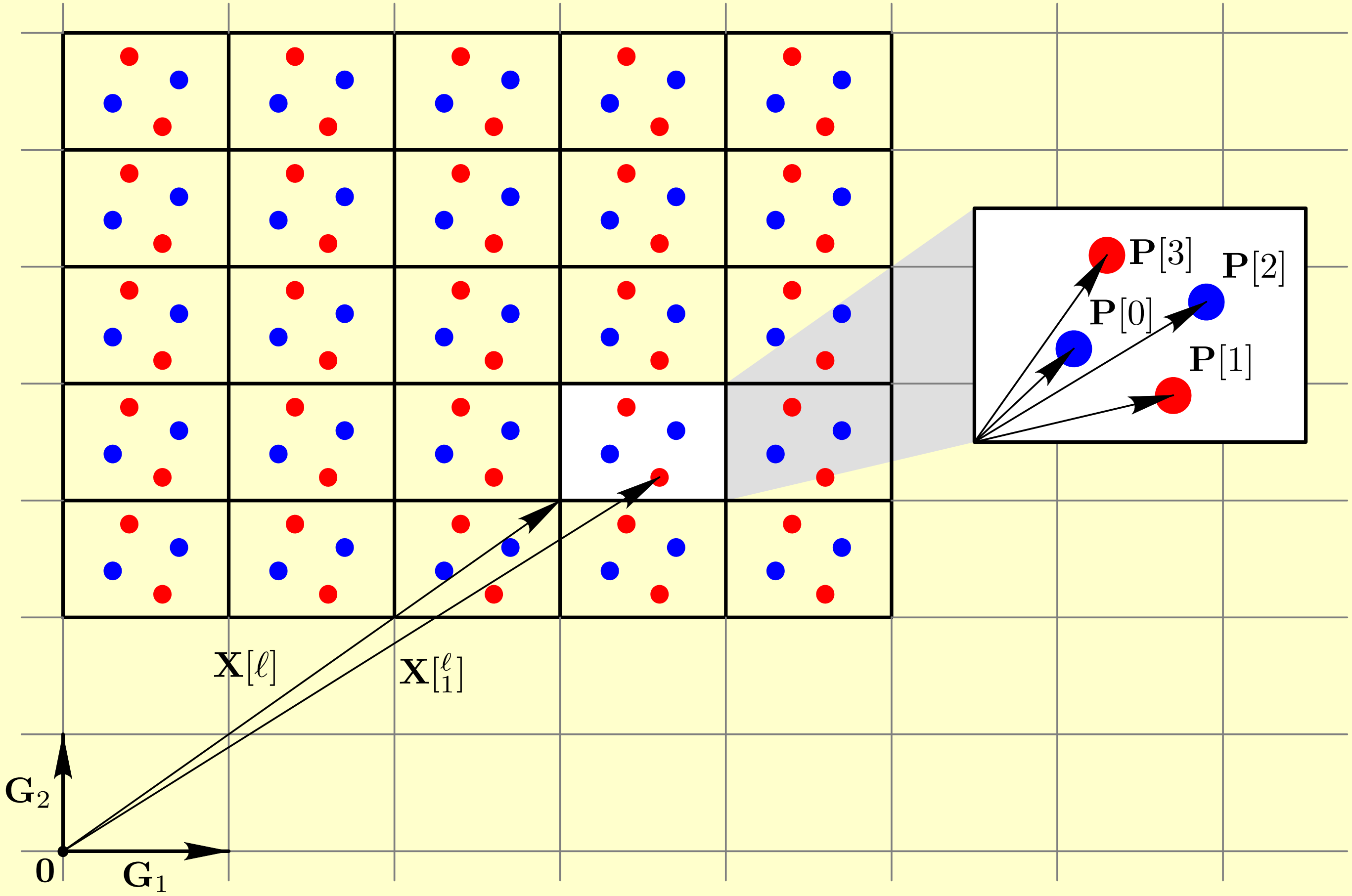
	r_0	r_θ	β	A	mass
aa	1	0	4	1	1
bb	1.060	0.010	7	1	0.816
ab	1.026	0.005	5.5	1	N/A







Multilattice (Cauchy-Born Kinematics)



$\mathbf{G}_i$ – ref. lattice basis

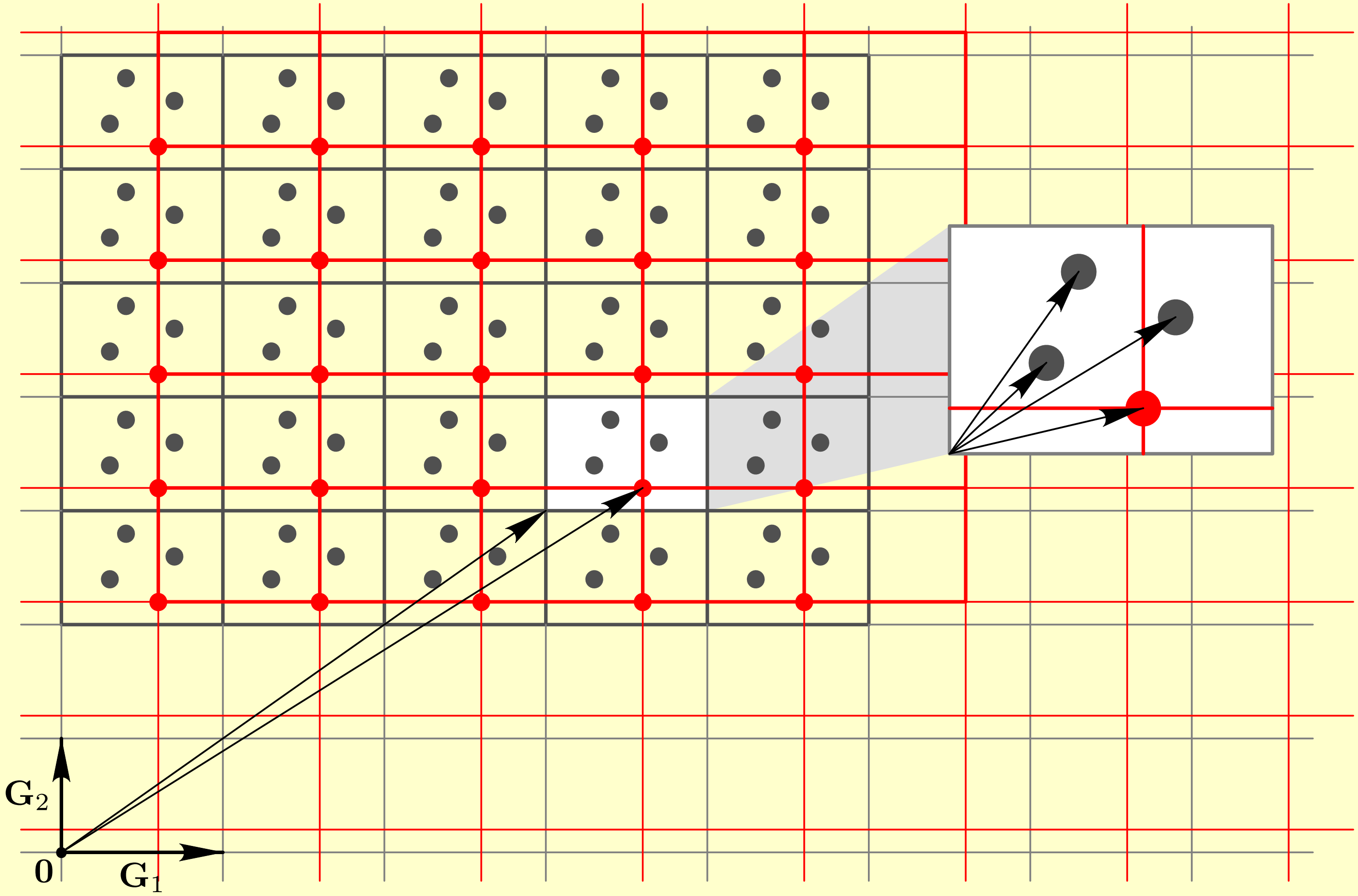
$\mathbf{X}[\ell]$ – unit-cell ref. pos.

$\mathbf{X}\begin{bmatrix}\ell\\\alpha\end{bmatrix}$ – reference pos.

$\mathbf{P}[\alpha]$ – fractional pos.

$$\alpha = 0, 1, 2, 3$$

Multilattice (Cauchy-Born Kinematics)



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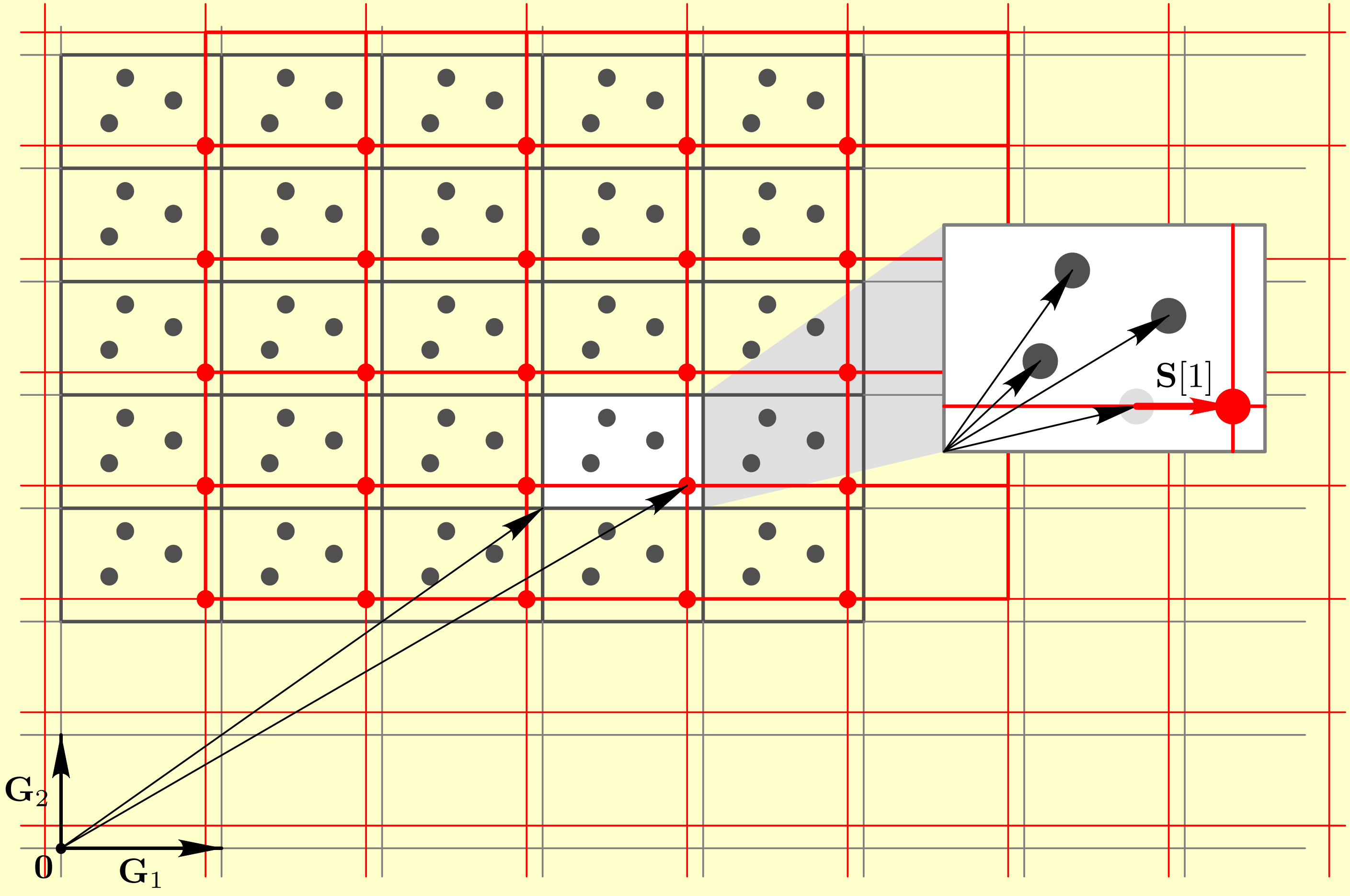

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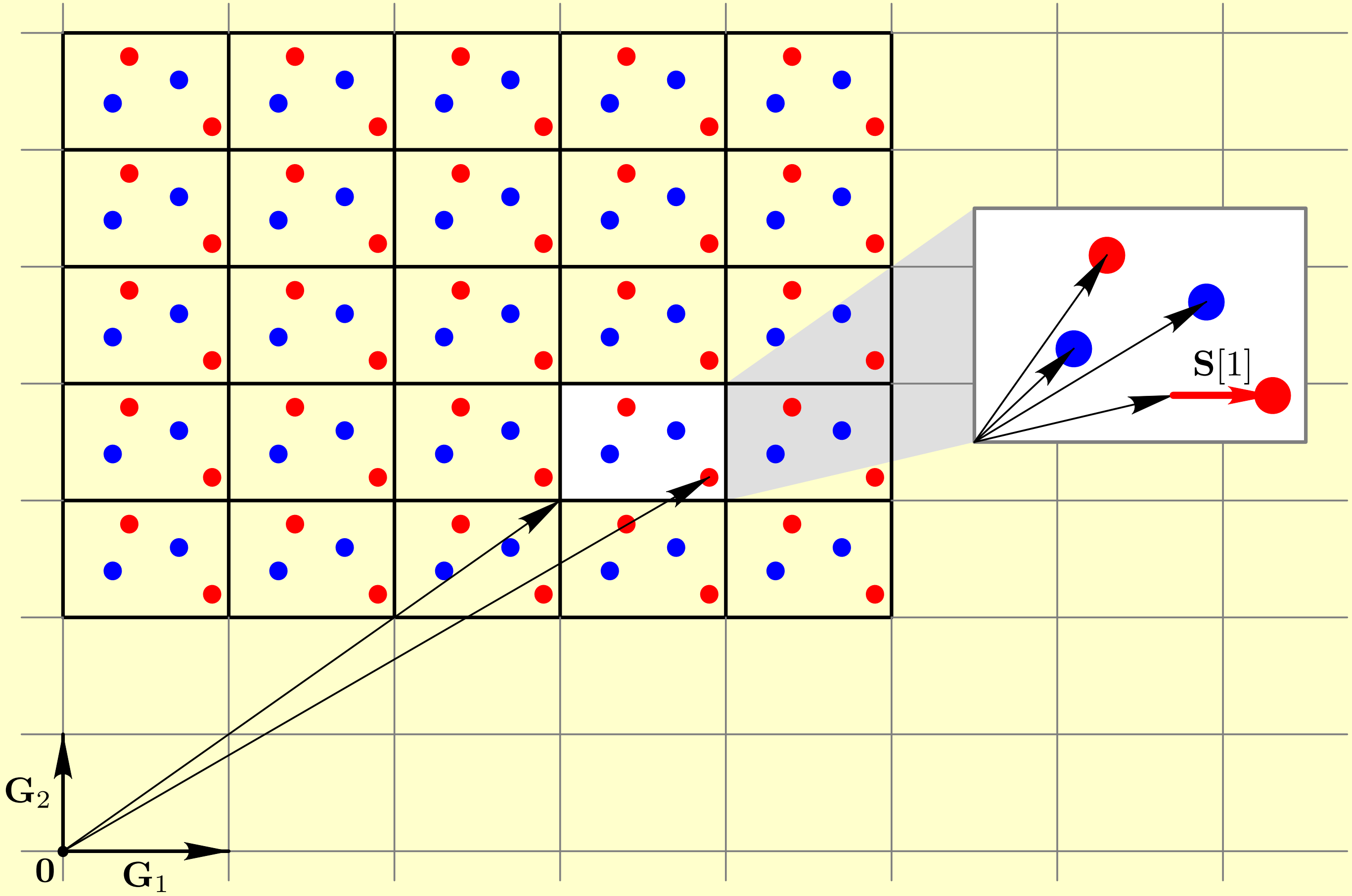
$\mathbf{S}[\alpha]$ – sub-lat. ref. shifts

Multilattice (Cauchy-Born Kinematics)



$\mathbf{G}_i$ – ref. lattice basis

$\mathbf{X}[\ell]$ – unit-cell ref. pos.

$\mathbf{X}\left[\begin{smallmatrix}\ell\\ \alpha\end{smallmatrix}\right]$ – reference pos.

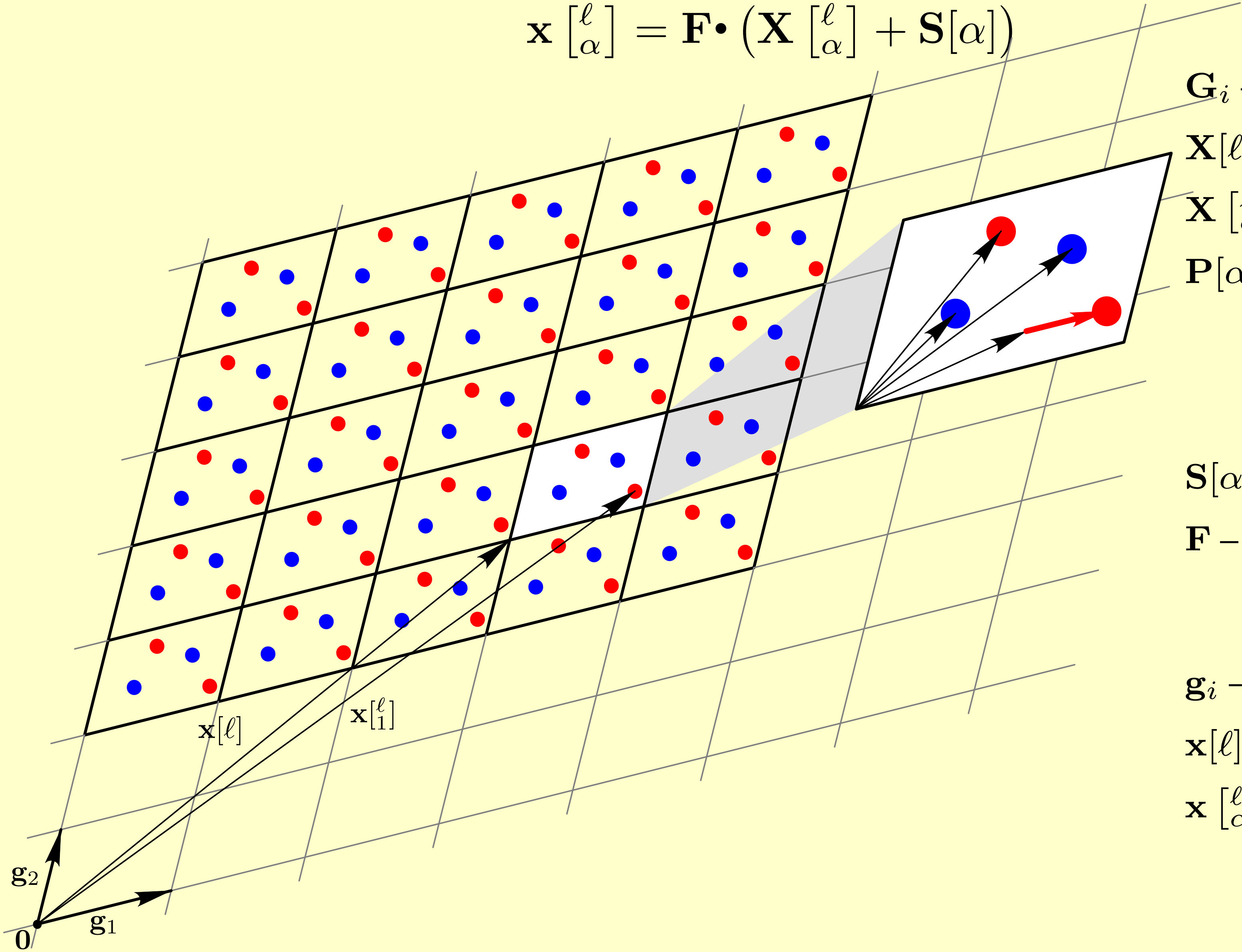
$\mathbf{P}[\alpha]$ – fractional pos.

$$\alpha = 0, 1, 2, 3$$

$\mathbf{S}[\alpha]$ – sub-lat. ref. shifts

Multilattice (Cauchy-Born Kinematics)

$$\mathbf{x}\begin{bmatrix}\ell\\\alpha\end{bmatrix} = \mathbf{F}\bullet\left(\mathbf{X}\begin{bmatrix}\ell\\\alpha\end{bmatrix} + \mathbf{S}[\alpha]\right)$$



$\mathbf{G}_i$ – ref. lattice basis

$\mathbf{X}[\ell]$ – unit-cell ref. pos.

$\mathbf{X}\begin{bmatrix}\ell\\\alpha\end{bmatrix}$ – reference pos.

$\mathbf{P}[\alpha]$ – fractional pos.

$\alpha = 0, 1, 2, 3$

$\mathbf{S}[\alpha]$ – sub-lat. ref. shifts

$\mathbf{F}$ – uniform deformation

$\mathbf{g}_i$ – current lattice basis

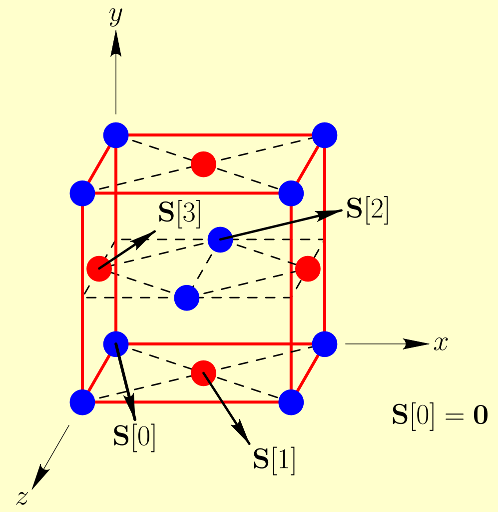
$\mathbf{x}[\ell]$ – unit-cell current pos.

$\mathbf{x}\begin{bmatrix}\ell\\\alpha\end{bmatrix}$ – current pos.

Multilattice Model & Stress-free Equilibrium

$\mathbf{X}\begin{bmatrix}\ell\\ \alpha\end{bmatrix}$ — reference position vector of atom α in unit cell ℓ

$\mathbf{S}[\alpha]$ — displacement vector of atom α (sub-lattice)
$\alpha = 0, 1, 2, 3$



- Current position vector (Cauchy-Born kinematics, $\alpha = 0, 1, 2, 3$)

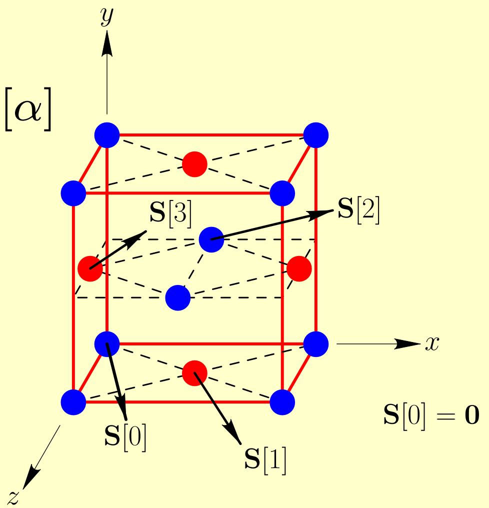
$$\mathbf{x}\begin{bmatrix}\ell\\ \alpha\end{bmatrix} = \mathbf{F}\bullet\left(\mathbf{X}\begin{bmatrix}\ell\\ \alpha\end{bmatrix} + \mathbf{S}[\alpha]\right)$$

- Energy density

$$\widetilde{W}(\mathbf{u};\theta) = \frac{1}{2V}\sum_{\alpha'}\sum_{\left[\begin{smallmatrix}\ell\\ \alpha\end{smallmatrix}\right]}\phi_{\alpha\alpha'}\left(r\begin{bmatrix}\ell & 0\\ \alpha & \alpha'\end{bmatrix};\theta\right)$$

$$\mathbf{u} \equiv \{\mathbf{F}, \mathbf{S}[1], \mathbf{S}[2], \mathbf{S}[3]\}, \qquad r\begin{bmatrix}\ell & \ell'\\ \alpha & \alpha'\end{bmatrix} = \left\|\mathbf{x}\begin{bmatrix}\ell\\ \alpha\end{bmatrix} - \mathbf{x}\begin{bmatrix}\ell'\\ \alpha'\end{bmatrix}\right\|$$

Multilattice Model & Stress-free Equilibrium



- Equilibrium: 15 DOFs — 6 from $\mathbf{U} = \mathbf{U}^T$ and 9 from $\mathbf{S}[\alpha]$

$$\frac{\partial \widetilde{W}}{\partial \mathbf{u}} = \mathbf{0} \begin{cases} \dfrac{\partial \widetilde{W}}{\partial \mathbf{U}} = \mathbf{0}, \\ \dfrac{\partial \widetilde{W}}{\partial \mathbf{S}[1]} = \mathbf{0}, \quad \dfrac{\partial \widetilde{W}}{\partial \mathbf{S}[2]} = \mathbf{0}, \quad \dfrac{\partial \widetilde{W}}{\partial \mathbf{S}[3]} = \mathbf{0}. \end{cases}$$

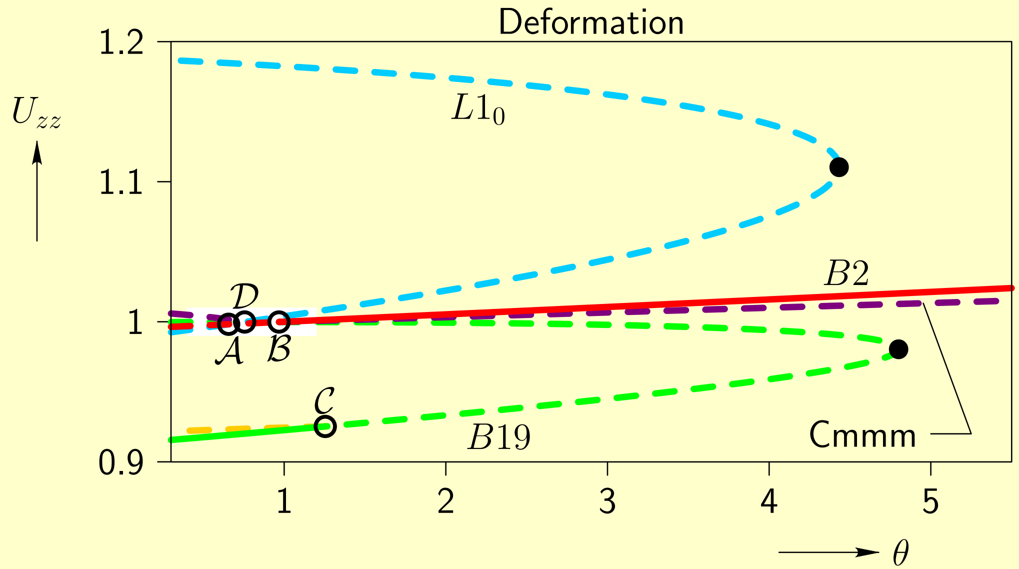
- Stability
  - Cauchy-Born stability (local energy minimizer):

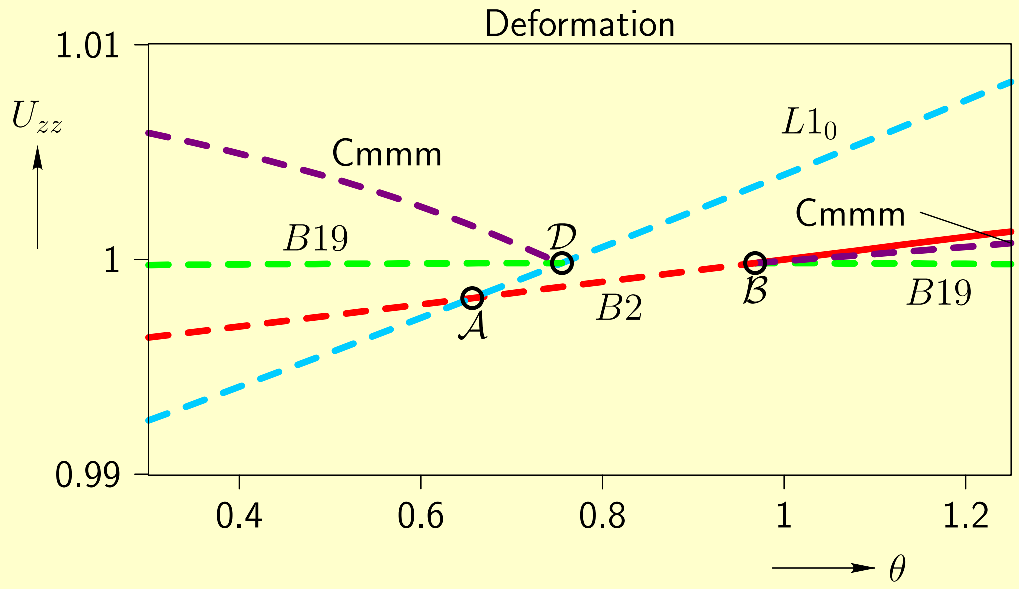
$$\delta\mathbf{u}\frac{\partial^2 \widetilde{W}}{\partial \mathbf{u}\partial \mathbf{u}}\delta\mathbf{u} > 0; \qquad \delta\mathbf{u} = \{\delta\mathbf{U}, \delta\mathbf{S}[1], \delta\mathbf{S}[2], \delta\mathbf{S}[3]\}, \ \delta\mathbf{U} = \delta\mathbf{U}^T.$$

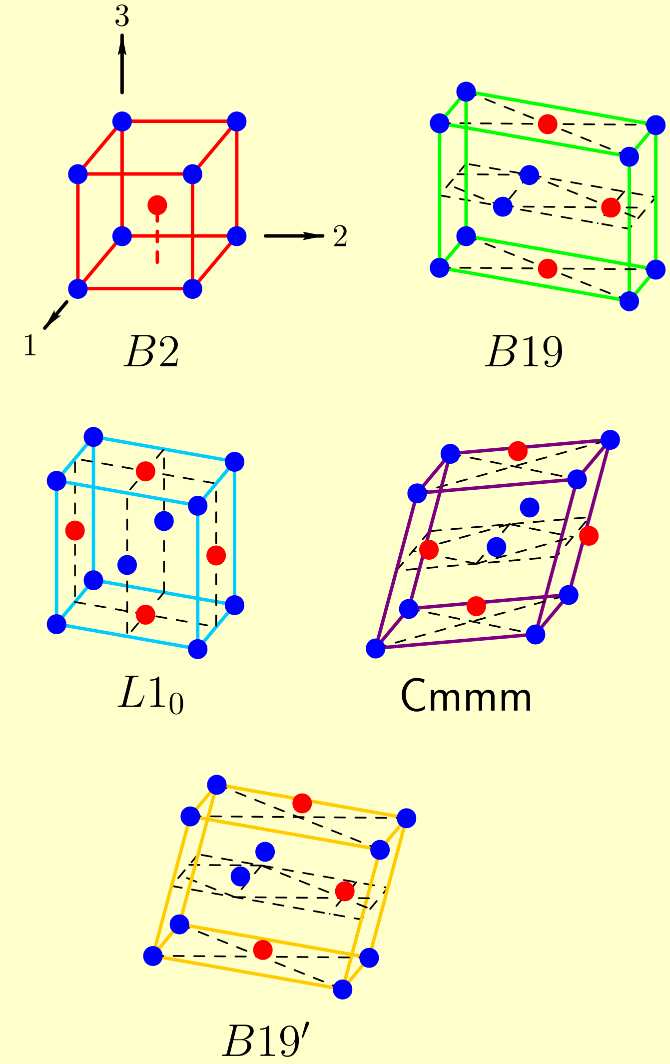
  - Phonon stability:

$$\left(\omega^{(q)}(\mathbf{k})\right)^2 > 0, \quad \forall \mathbf{k}, q.$$

4-Lattice Bifurcation Diagram







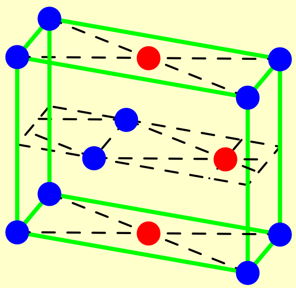
- Hysteretic proper Martensitic transformation between $B2$ & $B19$

Transformation Parameters

$$B2 \Longrightarrow B19$$

Martensitic Transformation

- Experimental right stretch tensor



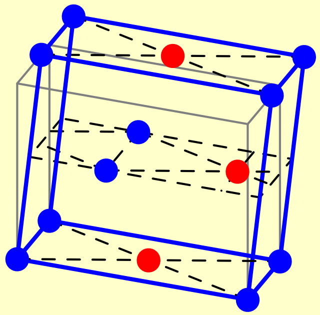
$$B19$$

$$\mathbf{U} = \begin{bmatrix} 1.024 & 0.0106 & 0 \\ 0.0106 & 1.024 & 0 \\ 0 & 0 & 0.9491 \end{bmatrix}$$

AuCd, (*Chang, Read (1951)*)

$$\mathbf{U} = \begin{bmatrix} 1.042 & 0.0194 & 0 \\ 0.0194 & 1.042 & 0 \\ 0 & 0 & 0.9178 \end{bmatrix}$$

CuAlNi, (*Otsuka, Shimizu (1974)*)

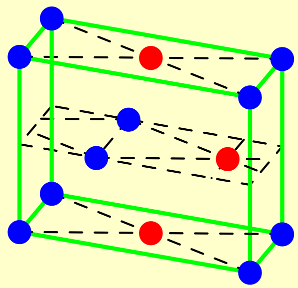


$$B19'$$

$$\mathbf{U} = \begin{bmatrix} 1.025 & 0.0620 & 0.0490 \\ 0.0620 & 1.025 & 0.0490 \\ 0.0490 & 0.0490 & 0.9587 \end{bmatrix}$$

NiTi, (*Otsuka et al. (1971)*)

- Simulated right stretch tensor ($\theta = 1.0$)



$$B19$$

$$\mathbf{U} = \begin{bmatrix} 1.045 & 0.0173 & 0 \\ 0.0173 & 1.045 & 0 \\ 0 & 0 & 0.9224 \end{bmatrix}$$

Computational Challenges

- Crystal structure stability
  - Robust stability criterion — phonon spectra
  - Efficient numerical evaluation of phonon spectra
- Efficient equilibrium path following
  - Reduced set of equations based on symmetry
  - Pseudo-arc-length method
- Determine behavior near bifurcation points
  - Identify all paths that emerge from a bifurcation point
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Direct Computation of Stability

- Compute all eigenvalues of $K = \dfrac{\partial^2 \widetilde{W}}{\partial \mathbf{u}\left[\begin{smallmatrix}\ell\\\alpha\end{smallmatrix}\right] \partial \mathbf{u}\left[\begin{smallmatrix}\ell\\\alpha\end{smallmatrix}\right]}$, $(3MN \times 3MN)$

  M—number of atoms per unit cell

  N—number of unit cells in crystal

$$\begin{bmatrix} * & * & * & \cdots \\ * & * & * & \cdots \\ * & * & * & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix} \Longrightarrow \begin{bmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \lambda_3 & \\ & & & \ddots \end{bmatrix}$$

  - Methods: SVD, LDU, Cholseky, Jacobi, Householder, etc.
  - Time complexity: $O\left([3MN]^3\right)$. Too slow for large N

Reduction to Block Diagonal Form

- In $3M \times 3M$ block form

$$K = \begin{bmatrix} \ddots & & & \\ & \left(K\begin{bmatrix} n-1 & n-1 \\ \alpha & \beta \end{bmatrix}\right) & \left(K\begin{bmatrix} n-1 & n \\ \alpha & \beta \end{bmatrix}\right) & \left(K\begin{bmatrix} n-1 & n+1 \\ \alpha & \beta \end{bmatrix}\right) & \\ & \left(K\begin{bmatrix} n & n-1 \\ \alpha & \beta \end{bmatrix}\right) & \left(K\begin{bmatrix} n & n \\ \alpha & \beta \end{bmatrix}\right) & \left(K\begin{bmatrix} n & n+1 \\ \alpha & \beta \end{bmatrix}\right) & \\ & \left(K\begin{bmatrix} n+1 & n-1 \\ \alpha & \beta \end{bmatrix}\right) & \left(K\begin{bmatrix} n+1 & n \\ \alpha & \beta \end{bmatrix}\right) & \left(K\begin{bmatrix} n+1 & n+1 \\ \alpha & \beta \end{bmatrix}\right) & \\ & & & & \ddots \end{bmatrix}$$

Reduction to Block Diagonal Form

- In $3M \times 3M$ block form

$$K = \begin{bmatrix} \ddots & & & & \\ & \left(K \begin{bmatrix} 0 & 0 \\ \alpha & \beta \end{bmatrix}\right) & \left(K \begin{bmatrix} 0 & 1 \\ \alpha & \beta \end{bmatrix}\right) & \left(K \begin{bmatrix} -1 & 1 \\ \alpha & \beta \end{bmatrix}\right) & \\ & \left(K^T \begin{bmatrix} 0 & 1 \\ \alpha & \beta \end{bmatrix}\right) & \left(K \begin{bmatrix} 0 & 0 \\ \alpha & \beta \end{bmatrix}\right) & \left(K \begin{bmatrix} 0 & 1 \\ \alpha & \beta \end{bmatrix}\right) & \\ & \left(K^T \begin{bmatrix} -1 & 1 \\ \alpha & \beta \end{bmatrix}\right) & \left(K^T \begin{bmatrix} 0 & 1 \\ \alpha & \beta \end{bmatrix}\right) & \left(K \begin{bmatrix} 0 & 0 \\ \alpha & \beta \end{bmatrix}\right) & \\ & & & & \ddots \end{bmatrix}$$

Translational periodicity (block-circulant matrix)

Reduction to Block Diagonal Form

- In $3M \times 3M$ block form

$$K = \begin{bmatrix} \ddots & & & & \\ & \left(K \begin{bmatrix} 0 & 0 \\ \alpha & \beta \end{bmatrix}\right) & \left(K \begin{bmatrix} 0 & 1 \\ \alpha & \beta \end{bmatrix}\right) & \left(K \begin{bmatrix} -1 & 1 \\ \alpha & \beta \end{bmatrix}\right) & \\ & \left(K^T \begin{bmatrix} 0 & 1 \\ \alpha & \beta \end{bmatrix}\right) & \left(K \begin{bmatrix} 0 & 0 \\ \alpha & \beta \end{bmatrix}\right) & \left(K \begin{bmatrix} 0 & 1 \\ \alpha & \beta \end{bmatrix}\right) & \\ & \left(K^T \begin{bmatrix} -1 & 1 \\ \alpha & \beta \end{bmatrix}\right) & \left(K^T \begin{bmatrix} 0 & 1 \\ \alpha & \beta \end{bmatrix}\right) & \left(K \begin{bmatrix} 0 & 0 \\ \alpha & \beta \end{bmatrix}\right) & \\ & & & & \ddots \end{bmatrix}$$

$\Downarrow$ Translational periodicity (block-circulant matrix)
block-Fourier transform

$$\mathbb{K} = \begin{bmatrix} \ddots & & & & \\ & \left(\mathbb{K} \begin{bmatrix} k-1 & \\ \alpha & \beta \end{bmatrix}\right) & (0) & (0) & \\ & (0) & \left(\mathbb{K} \begin{bmatrix} k & \\ \alpha & \beta \end{bmatrix}\right) & (0) & \\ & (0) & (0) & \left(\mathbb{K} \begin{bmatrix} k+1 & \\ \alpha & \beta \end{bmatrix}\right) & \\ & & & & \ddots \end{bmatrix}$$

- $3M \times 3M$ block diagonal form $\Longrightarrow$ Time complexity: $O\left([3M]^3 N\right)$.

Computational Challenges

- Crystal structure stability
  - Robust stability criterion — phonon spectra
  - Efficient numerical evaluation of phonon spectra
- Efficient equilibrium path following
  - Reduced set of equations based on symmetry
  - Pseudo-arc-length method
- Determine behavior near bifurcation points
  - Identify all paths that emerge from a bifurcation point
  - Numerical implementation of asymptotic analysis
    - Projection operators

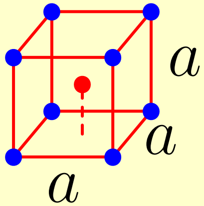
Following Equilibrium Paths

Solve a *reduced* set of equilibrium equations, e.g.,

- **Cubic Phase**

$$U_{11} = U_{22} = U_{33} = a,$$
$$U_{12} = U_{23} = U_{31} = 0.$$

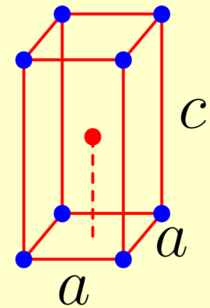
Solve: $\boxed{\dfrac{\partial \widetilde{W}}{\partial a} = 0.}$



- **Tetragonal Phase**

$$U_{33} = c, \quad U_{11} = U_{22} = a,$$
$$U_{12} = U_{23} = U_{31} = 0.$$

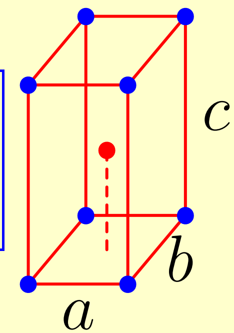
Solve: $\boxed{\dfrac{\partial \widetilde{W}}{\partial a} = 0, \quad \dfrac{\partial \widetilde{W}}{\partial c} = 0.}$



- **Orthorhombic Phase**

$$U_{11} = a, \quad U_{22} = b, \quad U_{33} = c,$$
$$U_{12} = U_{23} = U_{31} = 0.$$

Solve: $\boxed{\dfrac{\partial \widetilde{W}}{\partial a} = 0, \quad \dfrac{\partial \widetilde{W}}{\partial b} = 0, \quad \dfrac{\partial \widetilde{W}}{\partial c} = 0.}$

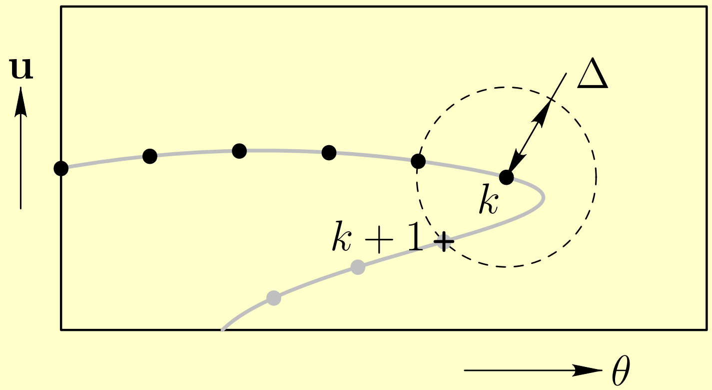


Advantages:

- Reduce computational effort
- Eliminate singularities near bifurcation points

Following Equilibrium Paths

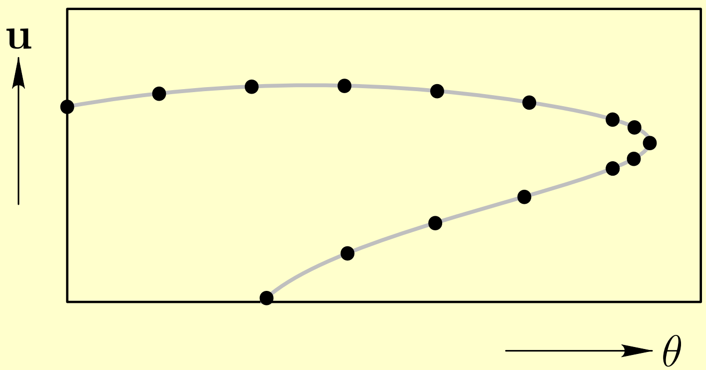
Problem: following an equilibrium path around a turning point



- Pseudo-arc-length method (Riks method)
  - known solution $\mathbf{u}(\theta_k)$
  - find solution $\mathbf{u}(\theta_{k+1})$ a "distance" Δ away
  - Augment equilibrium equations with "distance" constraint

$$\frac{\partial \widetilde{W}\left(\mathbf{u}(\theta_{k+1});\theta_{k+1}\right)}{\partial \mathbf{u}} = \mathbf{0}, \qquad \left\|\mathbf{u}(\theta_{k+1}) - \mathbf{u}(\theta_k)\right\|^2 + (\theta_{k+1} - \theta_k)^2 = \Delta^2$$

  - solve for θ_{k+1} and $\mathbf{u}(\theta_{k+1})$ simultaneously



- Also adaptively change Δ near turning points

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Asymptotic Bifurcation Analysis

- At a multiple bifurcation point, $(\mathbf{u}_c, \theta_c)$:

$$\left.\frac{\partial^2 \widetilde{W}}{\partial \mathbf{u}^2}\right|_c \text{ is singular with a null space of dimension } H \geq 2.$$

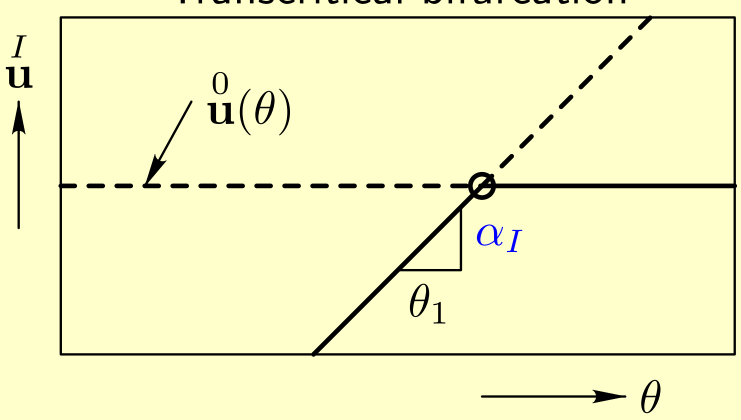
- Following *Triantafyllidis & Peek (1992),* (bifurcation amplitude parameter ξ)

$$\theta(\xi) = \theta_c + \theta_1 \xi + \theta_2 \frac{\xi^2}{2} + O\left(\xi^3\right),$$

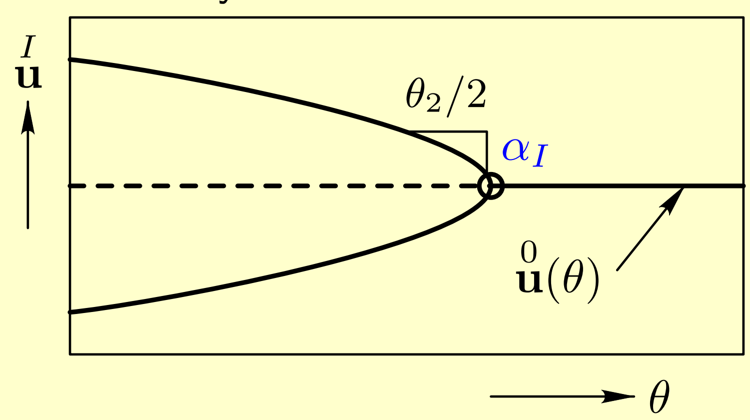
$$\mathbf{u}(\xi) = \overset{0}{\mathbf{u}}(\theta(\xi)) + \left(\sum_{I=1}^{H} \alpha_I \overset{I}{\mathbf{u}}\right) \xi + \left(\sum_{I,J=1}^{H} \alpha_I \alpha_J \overset{IJ}{\mathbf{v}}\right) \frac{\xi^2}{2} + O\left(\xi^3\right),$$

where $\left\{\overset{1}{\mathbf{u}}, \ldots, \overset{H}{\mathbf{u}}\right\}$ is an O.N. basis for the null space of $\left.\frac{\partial^2 \widetilde{W}}{\partial \mathbf{u}^2}\right|_c$.

Transcritical bifurcation



Symmetric bifurcation

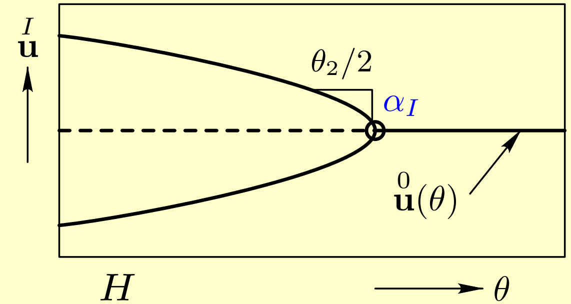


Numerical Asymptotic Bifurcation Analysis

Substitute into equilibrium equations $\frac{\partial \widetilde{W}}{\partial \mathbf{u}} = \mathbf{0}$, expand, and collect L.O.T.

- For *symmetric* bifurcation: $\left(\left. \frac{\partial^3 \widetilde{W}}{\partial \mathbf{u}^3} \right|_c \overset{I}{\mathbf{u}}\overset{J}{\mathbf{u}}\overset{K}{\mathbf{u}} \right) \equiv 0$

Symmetric bifurcation



$$\sum_{J,K,L=1}^{H} \alpha_J \alpha_K \alpha_L \mathcal{E}_{IJKL} + 3\theta_2 \sum_{J=1}^{H} \alpha_J \mathcal{E}_{IJ\theta} = 0, \qquad \sum_{I=1}^{H} (\alpha_I)^2 = 1.$$

$$\mathcal{E}_{IJ\theta} \equiv \left. \left(\frac{d}{d\theta} \left(\frac{\partial^2 \widetilde{W}(\overset{0}{\mathbf{u}}(\theta);\theta)}{\partial \mathbf{u} \partial \mathbf{u}} \right) \right) \right|_c \overset{I}{\mathbf{u}}\overset{J}{\mathbf{u}},$$

$$\mathcal{E}_{IJKL} \equiv \left. \frac{\partial^4 \widetilde{W}}{\partial \mathbf{u}^4} \right|_c \overset{J}{\mathbf{u}}\overset{K}{\mathbf{u}}\overset{L}{\mathbf{u}}\overset{I}{\mathbf{u}} + \left. \frac{\partial^3 \widetilde{W}}{\partial \mathbf{u}^3} \right|_c \left(\overset{JK}{\mathbf{v}}\overset{L}{\mathbf{u}} + \overset{KL}{\mathbf{v}}\overset{J}{\mathbf{u}} + \overset{LJ}{\mathbf{v}}\overset{K}{\mathbf{u}} \right) \overset{I}{\mathbf{u}},$$

$$\boxed{\left. \frac{\partial^2 \widetilde{W}}{\partial \mathbf{u}^2} \right|_c \overset{IJ}{\mathbf{v}} = - \left. \frac{\partial^3 \widetilde{W}}{\partial \mathbf{u}^3} \right|_c \overset{I}{\mathbf{u}}\overset{J}{\mathbf{u}}}$$

- Fredholm alternative guarantees a unique $\overset{IJ}{\mathbf{v}}$

Need $\overset{IJ}{\mathbf{v}}$:
$$\left.\frac{\partial^2 \widetilde{W}}{\partial \mathbf{u}^2}\right|_c \overset{IJ}{\mathbf{v}} = -\left.\frac{\partial^3 \widetilde{W}}{\partial \mathbf{u}^3}\right|_c \overset{I}{\mathbf{u}}\overset{J}{\mathbf{u}}$$

- Generate an O.N. basis for $\mathbb{R}^n$ by diagonalizing $\left.\dfrac{\partial^2 \widetilde{W}}{\partial \mathbf{u}^2}\right|_c \in \mathbb{R}^n \times \mathbb{R}^n$

$$\mathcal{N} = \mathrm{Span}\left\{\overset{1}{\mathbf{u}}, \ldots, \overset{H}{\mathbf{u}}\right\}, \qquad \mathcal{N}^\perp = \mathrm{Span}\left\{\overset{1}{\mathbf{v}}, \ldots, \overset{n-H}{\mathbf{v}}\right\}$$

- Projection operator $[Q_{Ij}] = [\overset{I}{v}_j] : \mathbb{R}^n \mapsto \mathcal{N}^\perp$

$$\underbrace{Q \left.\frac{\partial^2 \widetilde{W}}{\partial \mathbf{u}^2}\right|_c Q^T}_{\text{non-singular}} Q\overset{IJ}{\mathbf{v}} = -Q \left.\frac{\partial^3 \widetilde{W}}{\partial \mathbf{u}^3}\right|_c \overset{I}{\mathbf{u}}\overset{J}{\mathbf{u}}$$

- Solving gives

$$\overset{IJ}{\mathbf{v}} = \underbrace{\underbrace{-Q^T}_{n\times(n-H)} \underbrace{\left[Q \left.\frac{\partial^2 \widetilde{W}}{\partial \mathbf{u}^2}\right|_c Q^T\right]^{-1}}_{(n-H)\times(n-H)} \underbrace{Q \left.\frac{\partial^3 \widetilde{W}}{\partial \mathbf{u}^3}\right|_c \overset{I}{\mathbf{u}}\overset{J}{\mathbf{u}}}_{(n-H)\times 1}}_{n\times 1}.$$

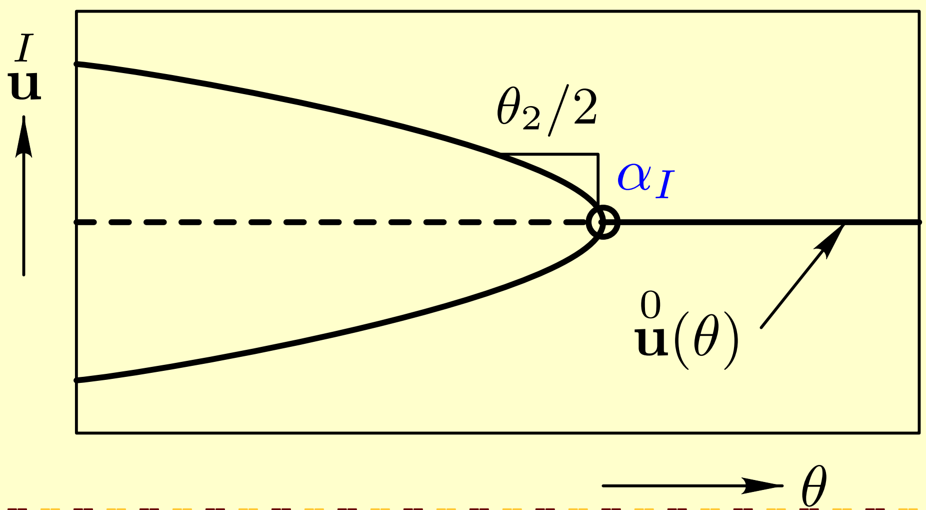
Numerical Asymptotic Bifurcation Analysis

- $\mathcal{E}_{IJ\theta}$, $\overset{IJ}{\mathbf{v}}$, and $\mathcal{E}_{IJKL}$ are obtained numerically
- *All* bifurcating equilibrium paths are found by solving

$$\sum_{J,K,L=1}^{H} \alpha_J \alpha_K \alpha_L \mathcal{E}_{IJKL} + 3\theta_2 \sum_{J=1}^{H} \alpha_J \mathcal{E}_{IJ\theta} = 0, \qquad \sum_{I=1}^{H} (\alpha_I)^2 = 1.$$

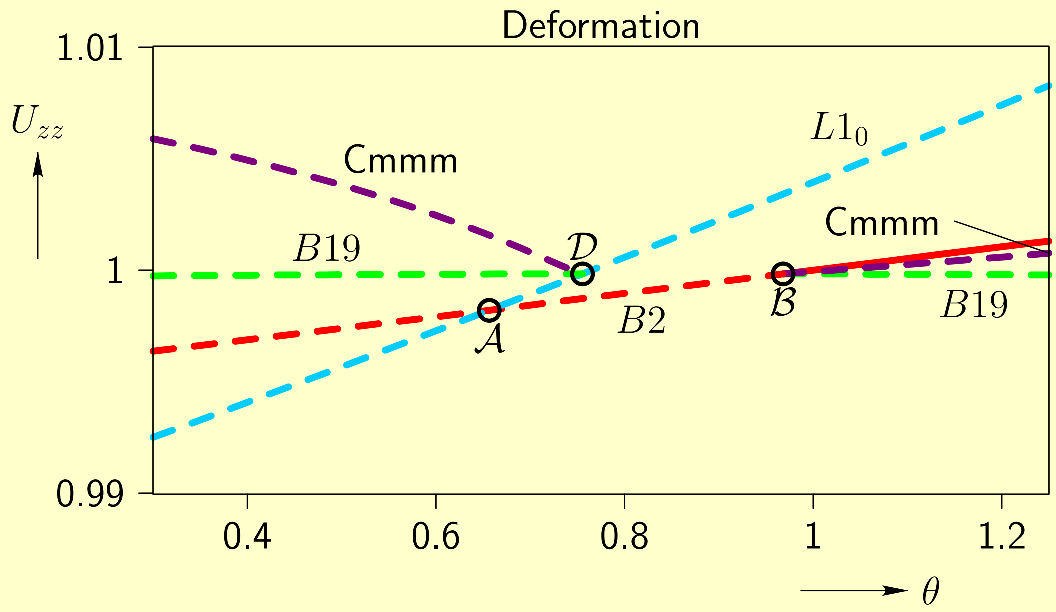
- In general there are $(3^H - 1)/2$ pairs of solutions (α_I, θ_2) and $(-\alpha_I, \theta_2)$
- Each *pair* of solutions corresponds to *one symmetric* equilibrium path

Symmetric bifurcation



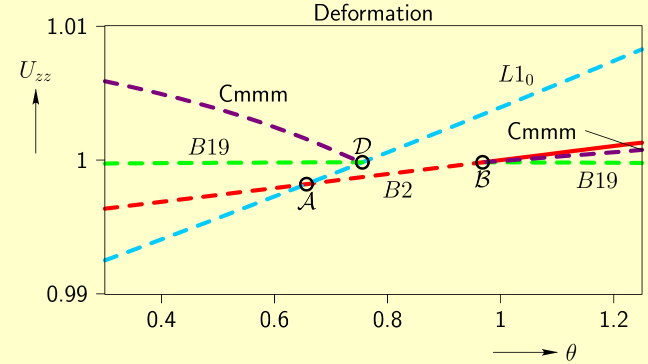
Example of Degree Two Bifurcation

- Bifurcation of degree two $(H = 2)$ at $\mathcal{B}$



Example of Degree Two Bifurcation

- Bifurcation of degree two ($H = 2$) at $\mathcal{B}$



- Basis for $\mathcal{N}$ (translation of certain crystal planes)

$$\overset{1}{\mathbf{u}} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0.6931 & 0 & 0 & 0.7203 & 0 & 0 & 0.0271 & 0 \end{bmatrix},$$

$$\overset{2}{\mathbf{u}} = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0.0271 & 0 & 0 & 0.7203 & 0 & 0 & 0.6931 & 0 & 0 \end{bmatrix}$$

- Resulting bifurcation equations $\qquad (\theta_1 = 0)$

$$-4849.2(\alpha_1)^3 - 19421\left(\alpha_1(\alpha_2)^2\right) + 3\theta_2(0.02425\alpha_1) = 0,$$

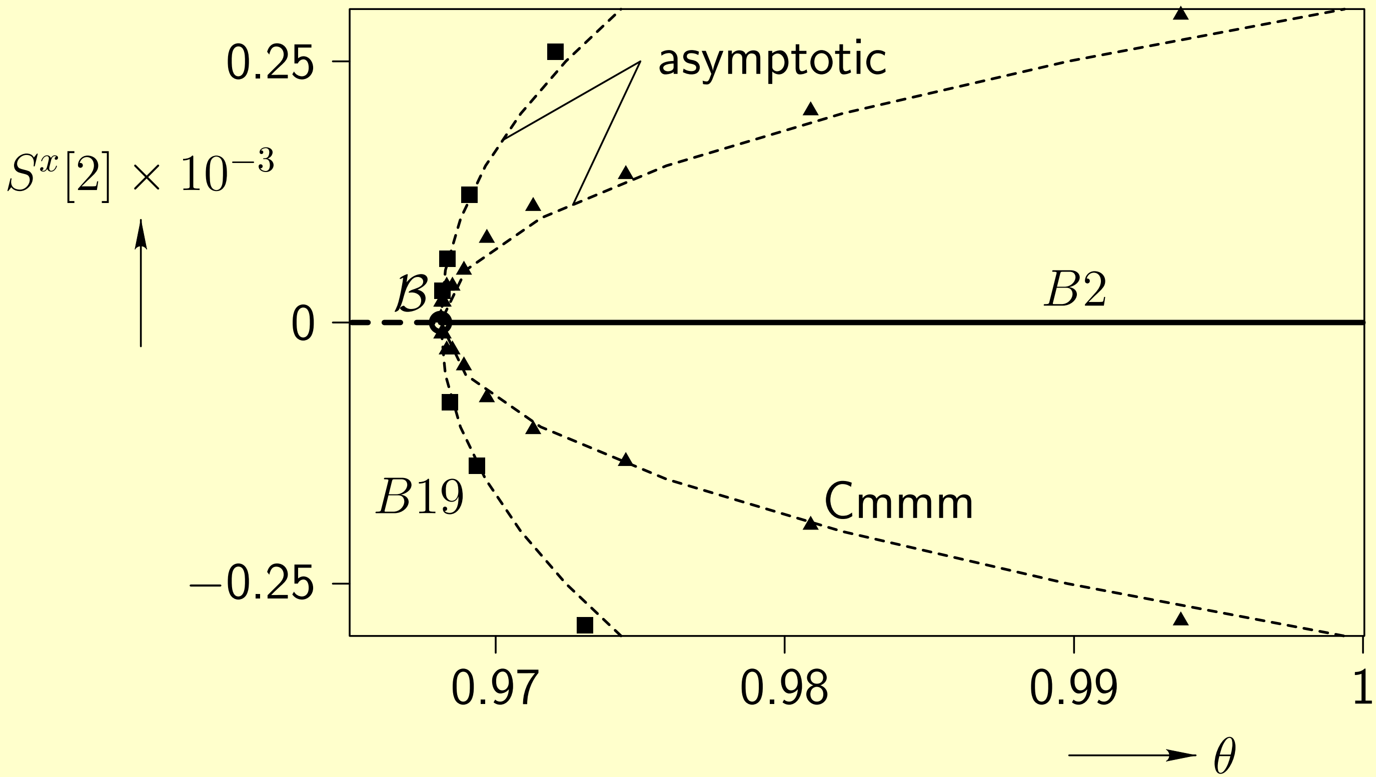
$$-19421\left((\alpha_1)^2\alpha_2\right) - 4849.2(\alpha_2)^3 + 3\theta_2(0.02425\alpha_2) = 0.$$

- Solutions (four pairs)

$$\begin{aligned} B19(1): &\quad \alpha_1 = 1,\ \alpha_2 = 0, &\quad \theta_2 = 66654,\\ B19(2): &\quad \alpha_1 = 0,\ \alpha_2 = 1, &\quad \theta_2 = 66654,\\ \mathrm{Cmmm}(1): &\quad \alpha_1 = 1,\ \alpha_2 = 1, &\quad \theta_2 = 333607,\\ \mathrm{Cmmm}(2): &\quad \alpha_1 = 1,\ \alpha_2 = -1, &\quad \theta_2 = 333607. \end{aligned}$$

Verification of Asymptotic Results

- Compare numerical and asymptotic results

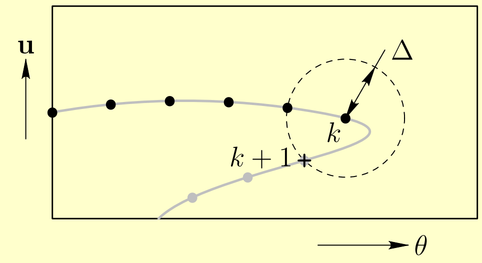


Summary & Conclusions

Numerical techniques for bifurcation investigation of atomistic material models

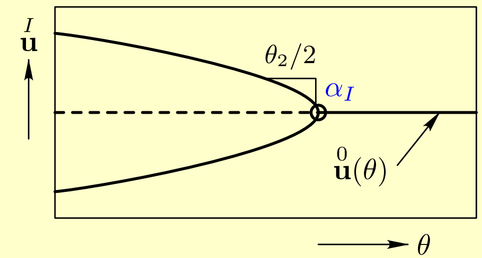
- Phonon spectra — important measure of crystal stability
  - Block-Fourier transform allows efficient phonon spectra computation
  - Time complexity $O\big((3M)^3N\big)$: linear in number of unit cells

- Efficient methods for following equilibrium paths
  - Reduce the number of equations by invoking symmetry
  - Pseudo-arc-length method



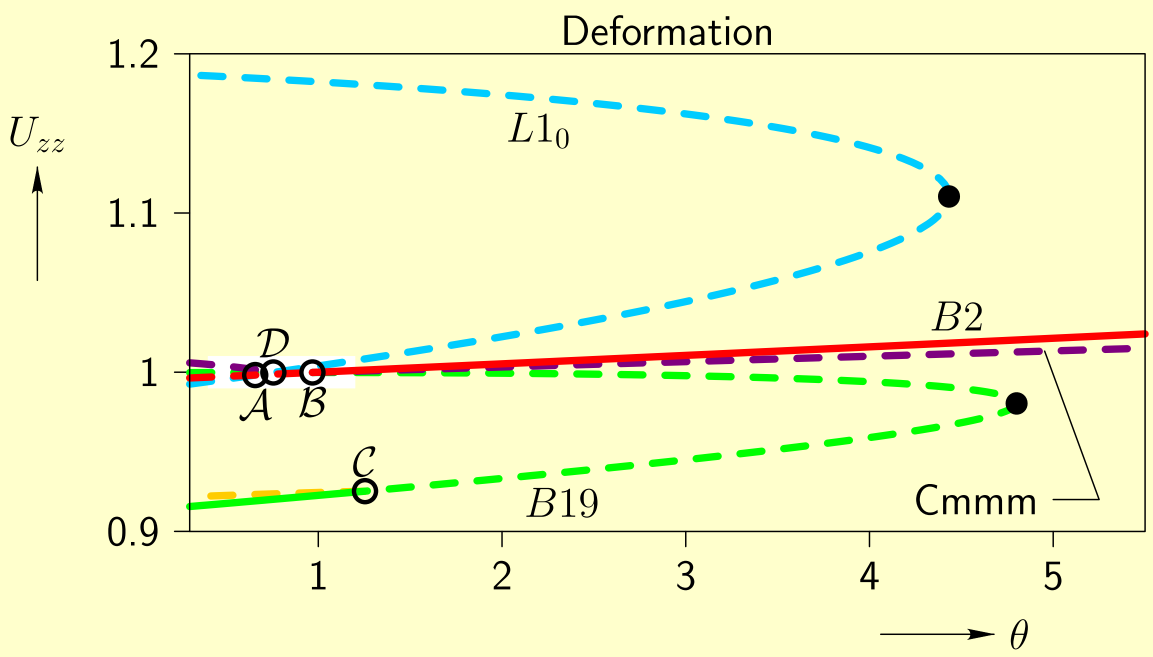
- Analyze behavior near bifurcation points
  - Numerically assisted asymptotic bifurcation investigation

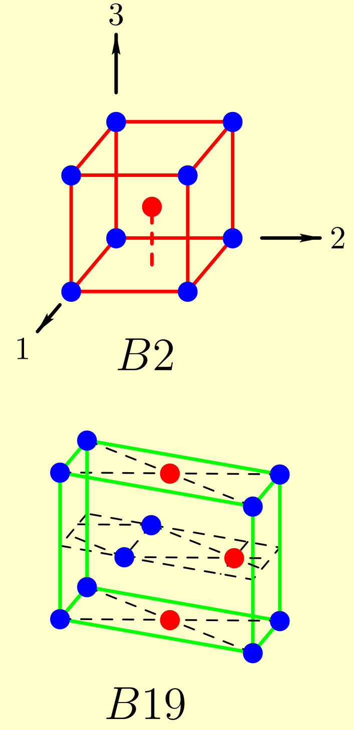
Symmetric bifurcation



Summary & Conclusions

- Used these computational techniques to study a new atomistic model
  - Temperature-dependent atomic-potentials
  - Cauchy-Born kinematics — uniform deformation & internal shifts





- Identified a hysteretic proper Martensitic transformation
  - Cubic austenite phase ($B2$ CsCl-type crystal)
  - Orthorhombic martensite phase ($B19$ crystal structure)
  - These structures are experimentally observed in SMA's such as AuCd, CuAlNi, and NiTiCu.