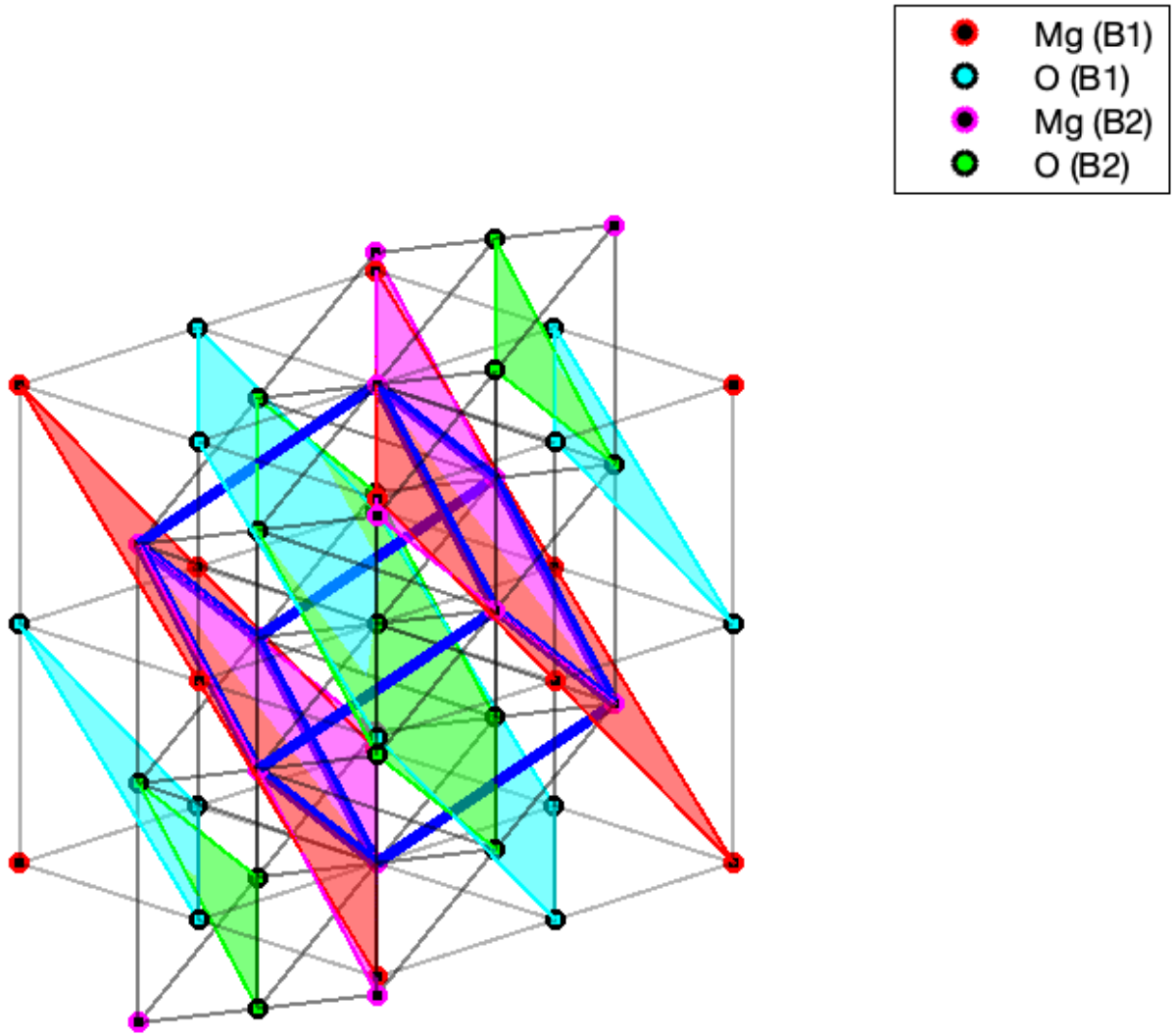
Kinetic transition pathway of pressure driven structural transformations: The case of magnesium oxide



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APS DPP GO07
Tues. Nov. 10, 2020

Summary

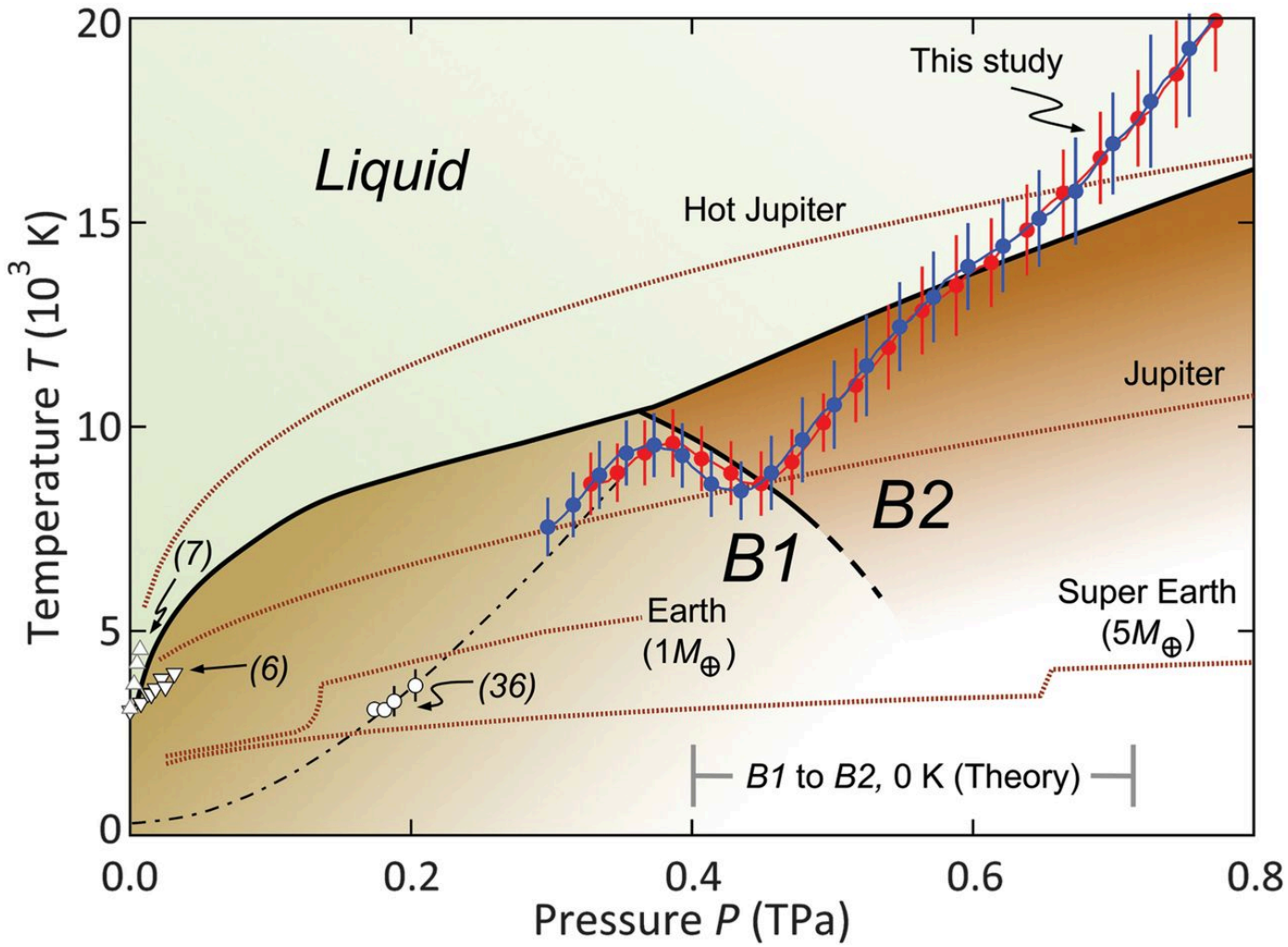
Geometry of the B1 to B2 transformation defines a crystal structure coordinate space.

- **Basis vectors connecting the B1 and B2 structures have been determined geometrically and are used to define a transformation matrix and structural coordinate space.**
- **Geometric multiplicity of the transformation is analyzed.**
- **Current/future work:**
  - **We are developing a predictive model to describe structural transformations as function of compression rate and 3D stress environment.**
  - **DFT analysis will be used to calculate the thermodynamic energy of crystal structures within the coordinate space. The thermodynamically optimal transition pathway will be identified.**

This material is based upon work supported by the Department of Energy National Nuclear Security Administration under Award Number DE-NA0003856.

Background

Knowing the process of the B1 to B2 transofrmation of MgO is important for HEDS.

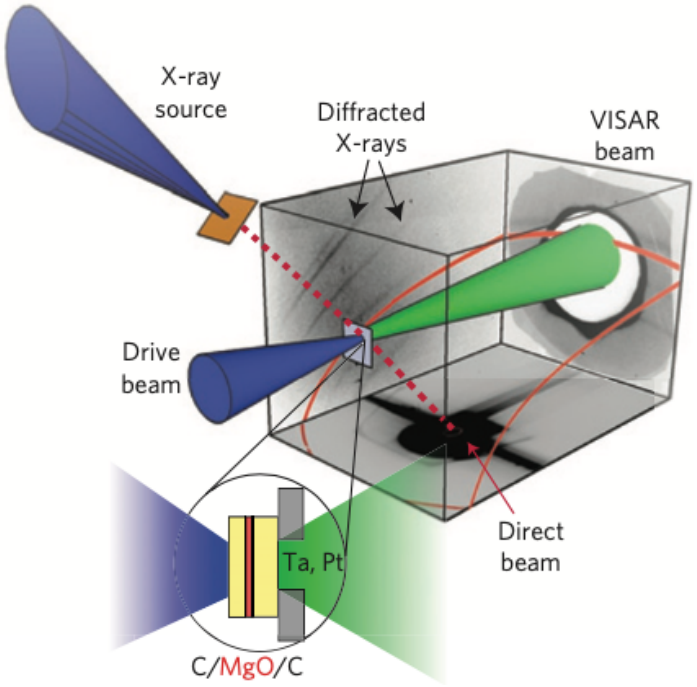


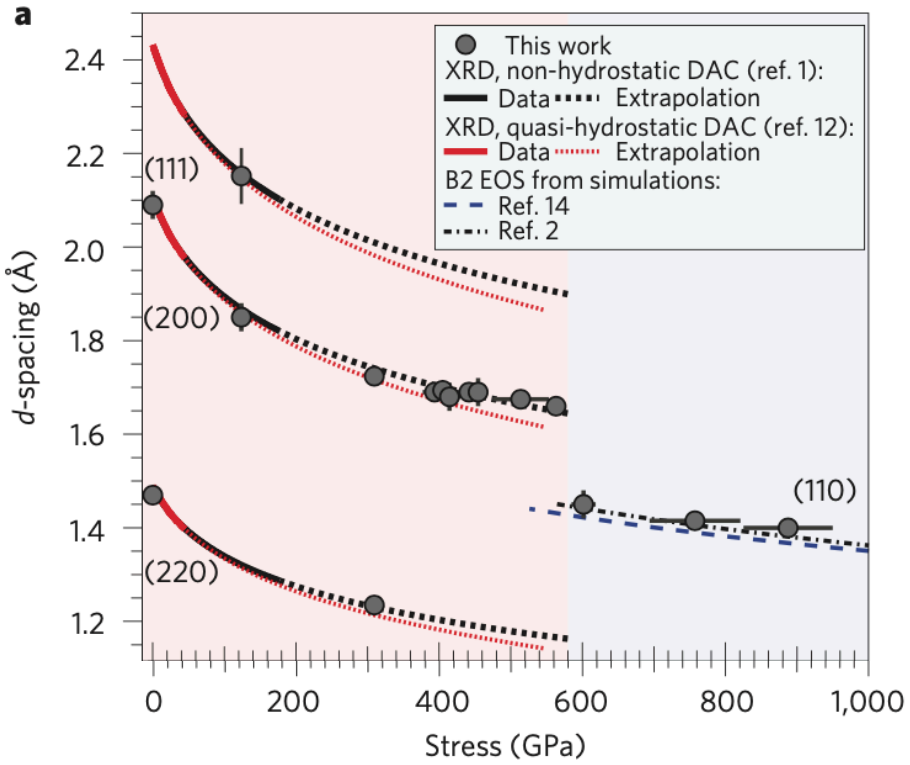
Magnesium oxide is an importnat window material in dynamic shock experiments, a pressure standard in DAC experiments, and a fundamental planet forming mineral.

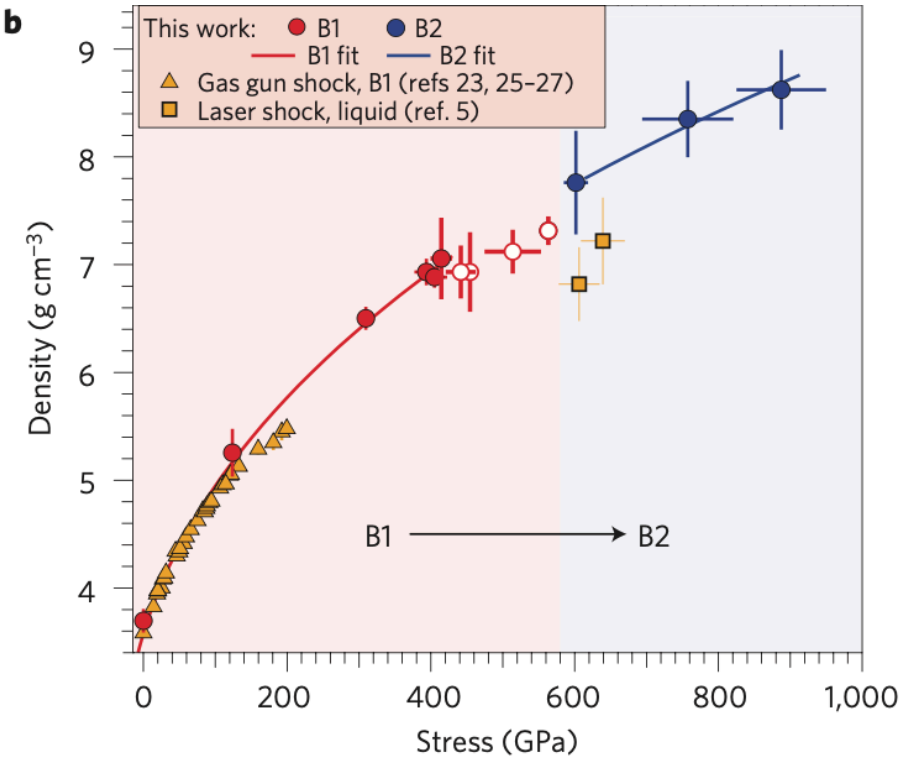
R. McWilliams , et al. *Science* 338, 1330 (2012)

Motivation

The high pressure MgO B1 to B2 structural transition pathway is unknown.



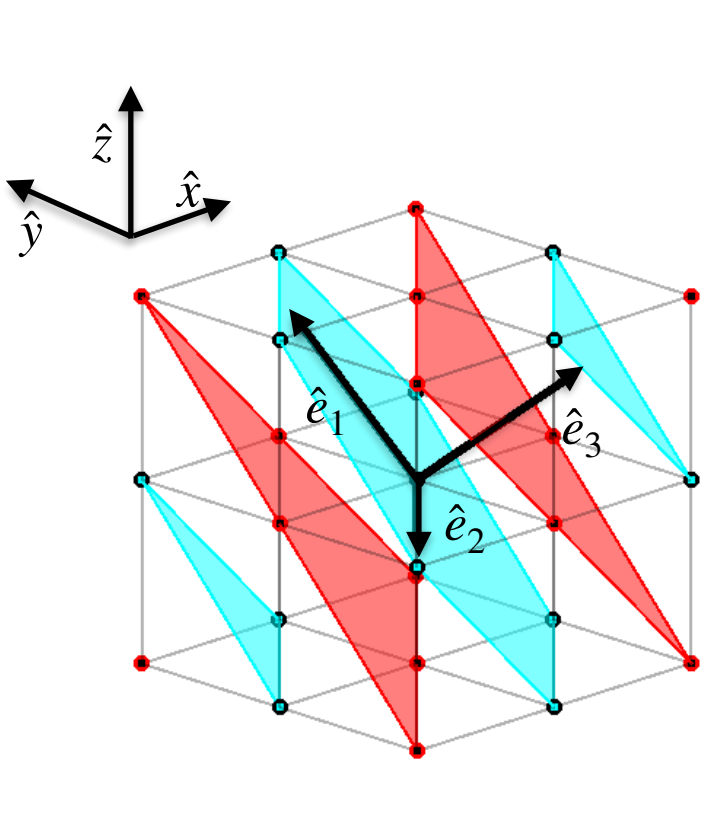


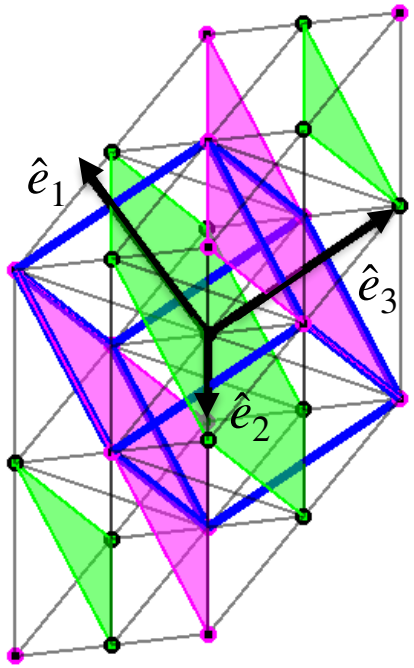


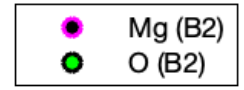
Ramp compression experiments have shown direct evidence of the MgO B1 to B2 transformation, intermediate data points remain unexplained.

F. Coppari, et al. *Nature Geoscience* 6, 926 (2013).

Transformation basis vectors connect the B1 and B2 structures.







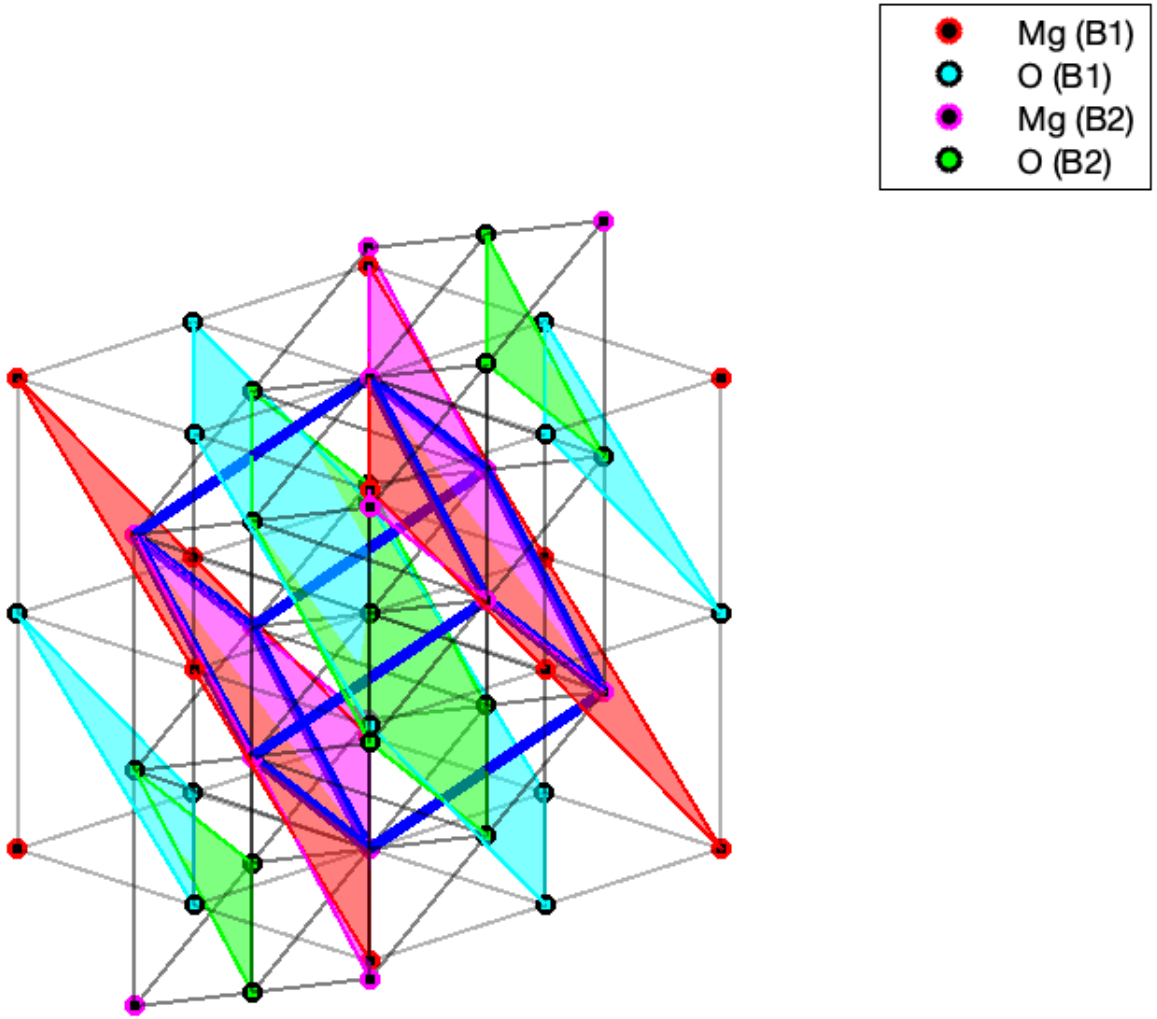
$$\hat{e}_1 = \frac{-1}{\sqrt{6}}\hat{x} + \frac{1}{\sqrt{6}}\hat{y} + \frac{2}{\sqrt{6}}\hat{z}$$

$$\hat{e}_2 = \frac{-1}{\sqrt{2}}\hat{x} - \frac{1}{\sqrt{2}}\hat{y}$$

$$\hat{e}_3 = \frac{1}{\sqrt{3}}\hat{x} - \frac{1}{\sqrt{3}}\hat{y} + \frac{1}{\sqrt{3}}\hat{z}$$

The B1 and B2 structures are related by scaling and shears along these orthogonal basis vectors.

A transformation matrix is defined by the basis vectors.



The matrix, X equals e_{ij}

$$X = \begin{bmatrix} -1/\sqrt{6} & 1/\sqrt{6} & 2/\sqrt{6} \\ -1/\sqrt{2} & -1/\sqrt{2} & 0 \\ 1/\sqrt{3} & -1/\sqrt{3} & 1/\sqrt{3} \end{bmatrix}$$

The B2 atomic position vectors can be obtained from the B1 atomic position vectors by multiplication of

$$X^T \begin{bmatrix} 2/3 & 0 & 0 \\ 0 & 2/\sqrt{3} & 0 \\ \sqrt{2}/3 & 0 & 1 \end{bmatrix} X$$

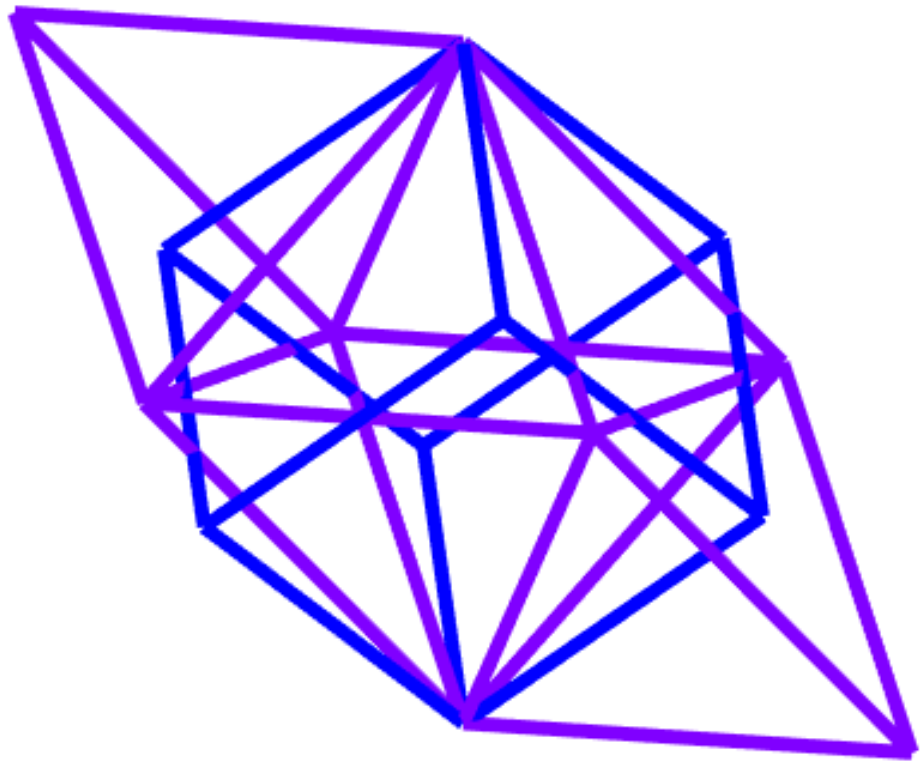
The coordination space connecting B1 and B2 is determined by the transformation matrix.

$$M = aX^T \begin{bmatrix} a_{11} & 0 & 0 \\ 0 & a_{22} & 0 \\ a_{31} & 0 & 1 \end{bmatrix} X$$

$$a_{11} \in [2/3,1]$$

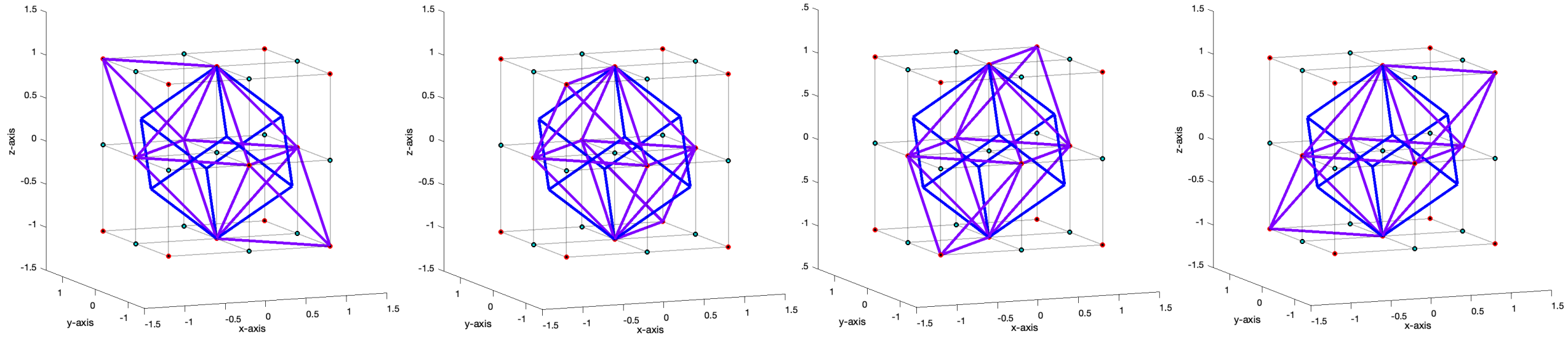
$$a_{22} \in [1,2/\sqrt{3}]$$

$$a_{31} \in [0,\sqrt{2}/3]$$



The goal is to use this coordinate space to determine the transition pathway with the lowest thermodynamic energy barrier, given the applied pressure.

This transformation basis has four fold multiplicity.



For a single crystal, a martensitic transformation could occur that would be characterized by this multiplicity.

We are building a theoretical model to predict structural transition pathways as a function of the compression rate and 3D stress environment.

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

stress — strain — elastic constants

$$\nabla \vec{u} = aX^T \begin{bmatrix} a_{11} & 0 & 0 \\ 0 & a_{22} & 0 \\ a_{31} & 0 & 1 \end{bmatrix} X$$

displacement vector

$$\vec{v} = \frac{\partial \vec{u}}{\partial t}$$

strain

$$\frac{1}{2}(\nabla \vec{u} + \nabla \vec{u}^T)$$

rotation

$$\frac{1}{2}(\nabla \vec{u} - \nabla \vec{u}^T)$$

rate of deformation

$$\frac{1}{2}(\nabla \vec{v} + \nabla \vec{v}^T)$$

rate of rotation

$$\frac{1}{2}(\nabla \vec{v} - \nabla \vec{v}^T)$$

W. Lai, D. Rubin, E. Krempl. *Introduction to Continuum Mechanics 4th ed.*, 3.7-3.13 (2009).

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