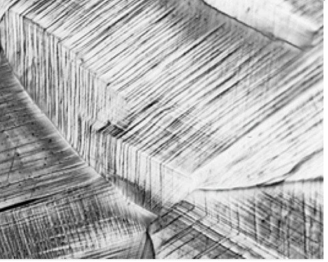
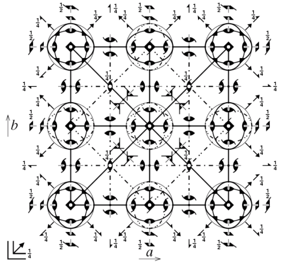
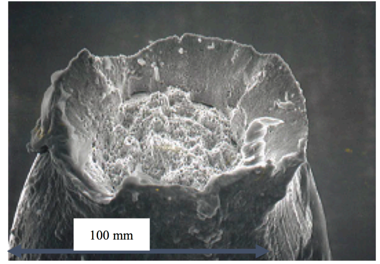
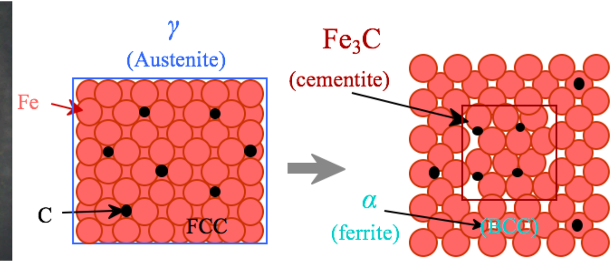








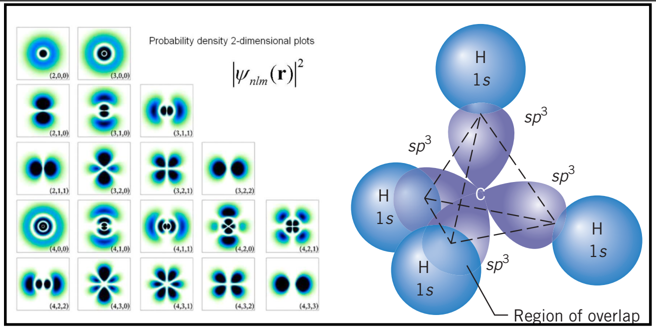
MEAM/MSE 507
Fundamentals of Materials

Prof. Jordan R. Raney

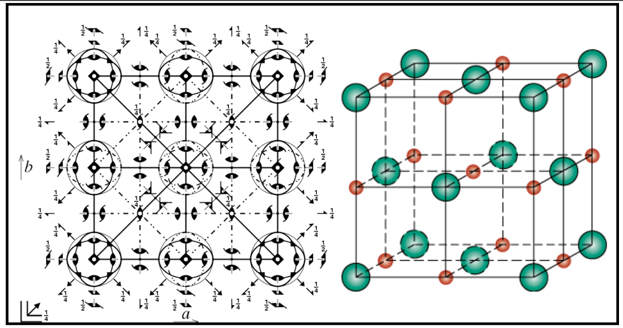
Week 4, Lecture 1: Foundations of crystallography: Symmetry operations

Asynchronous

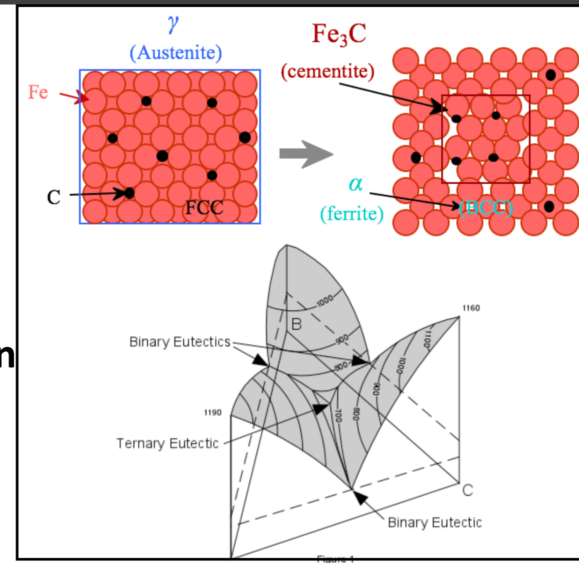
Major topics of the course



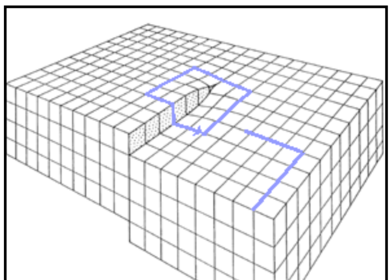
Quantum Mechanics and Bonding



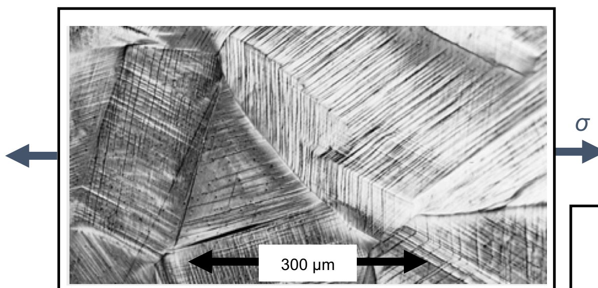
Symmetry, Crystallography, Diffraction



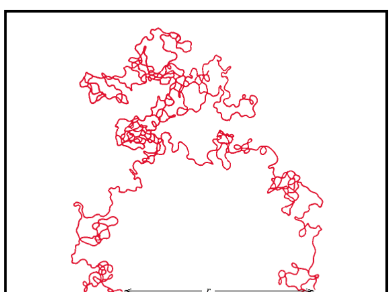
Phase Equilibrium



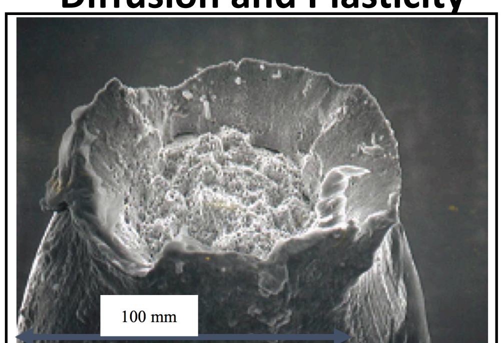
Defects



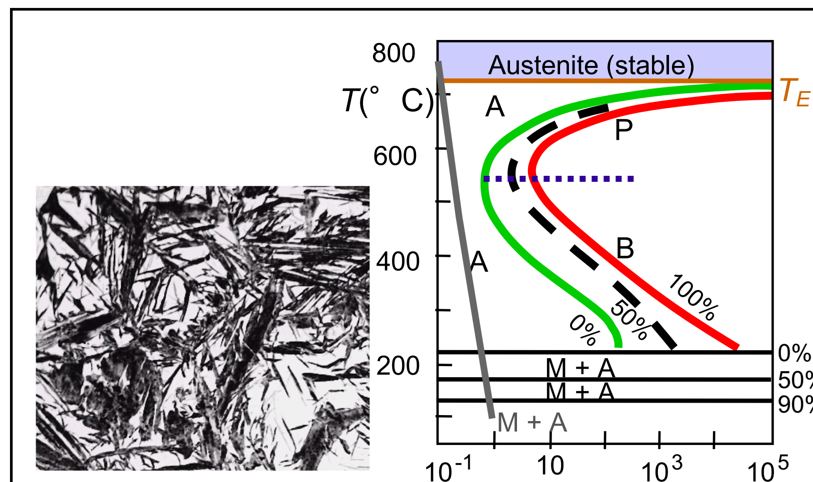
Diffusion and Plasticity



Polymers



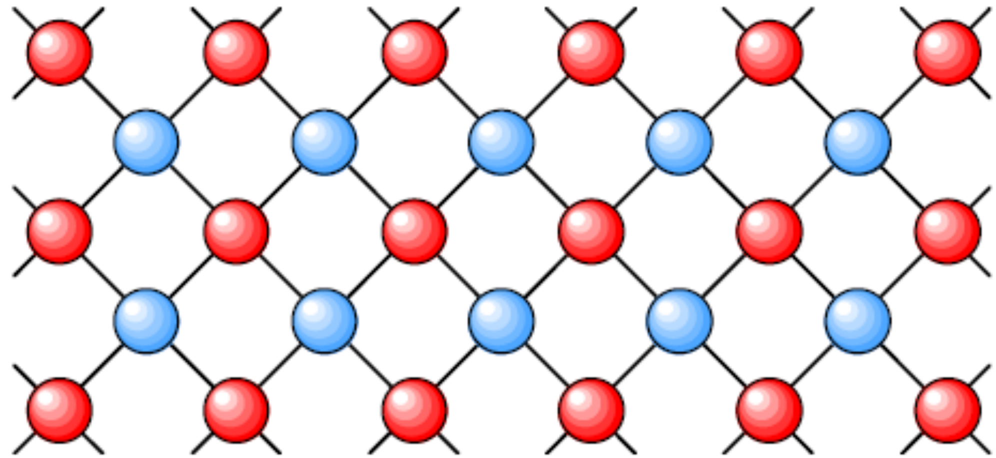
Failure



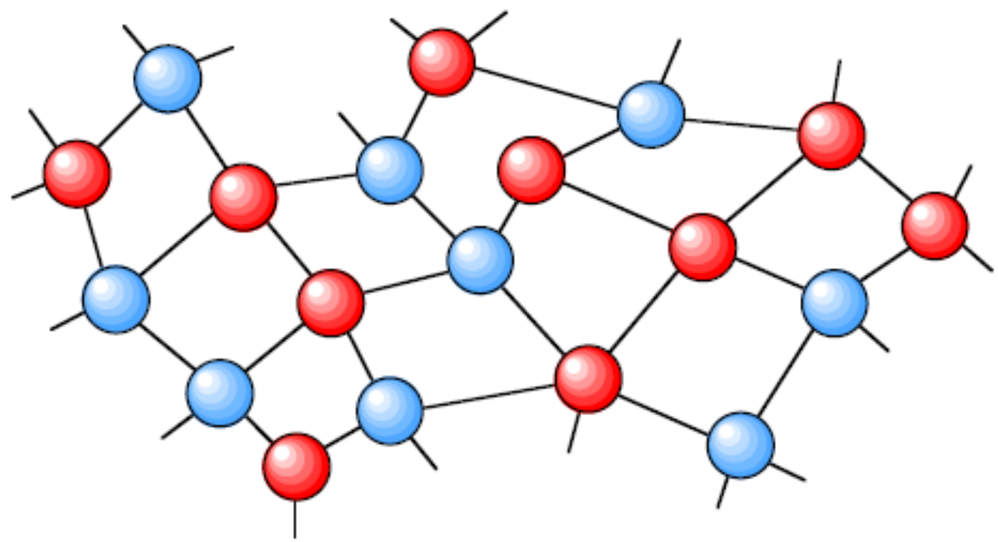
Phase Transformations

Crystal structure

Crystal
- Long range order
- Periodicity

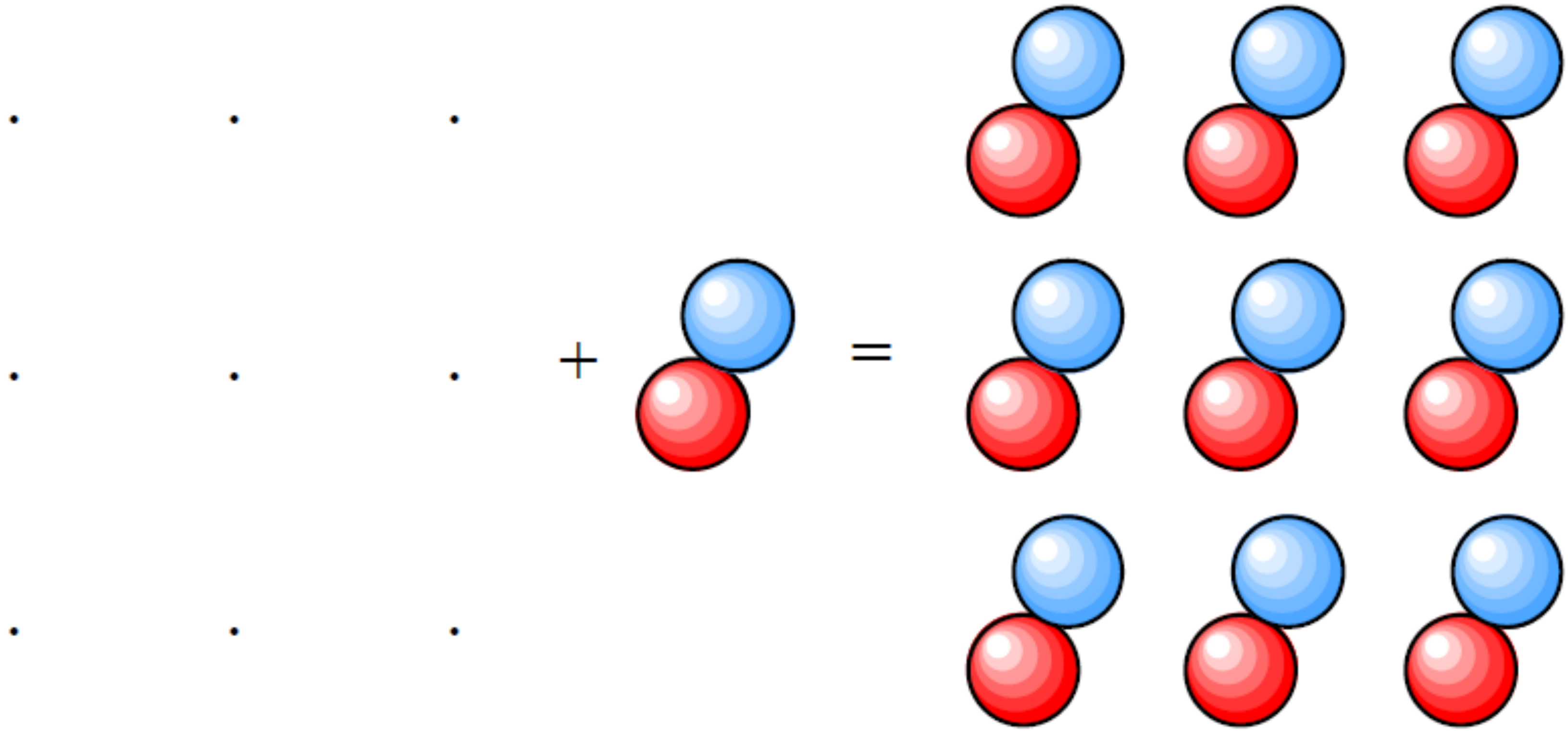


Amorphous/Glass
- No long range order
- Short range order



Crystal structure

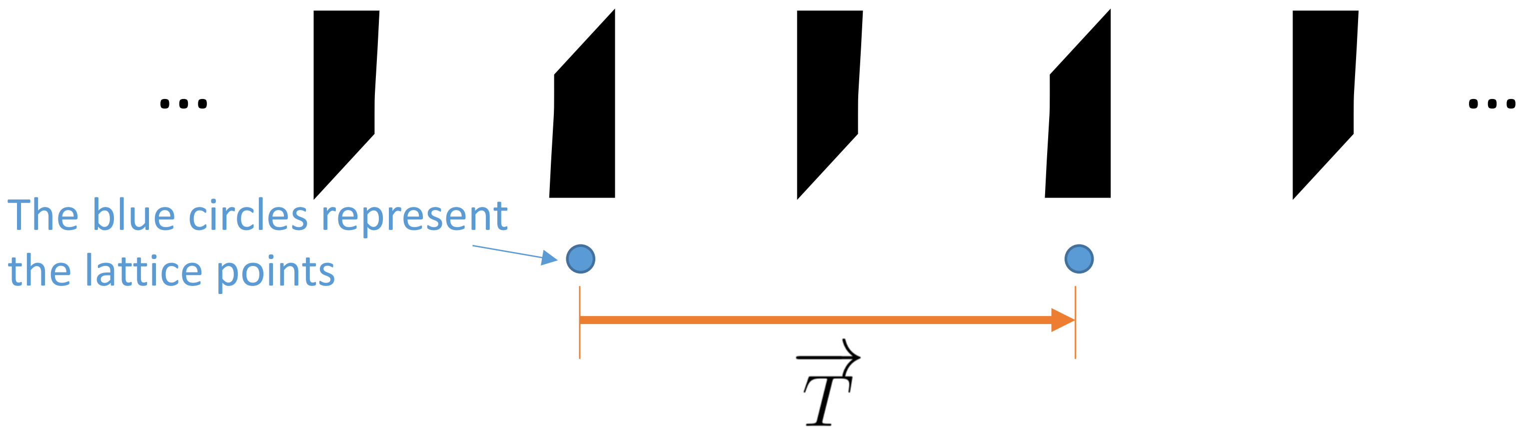
- A crystal has a space lattice and a basis (or “motif”)



- The space lattice tells us how the structure repeats
- The basis tells us what repeats

Symmetry

Imagine that this repeating pattern of chiral "motifs" extends forever in both directions (1D lattice):



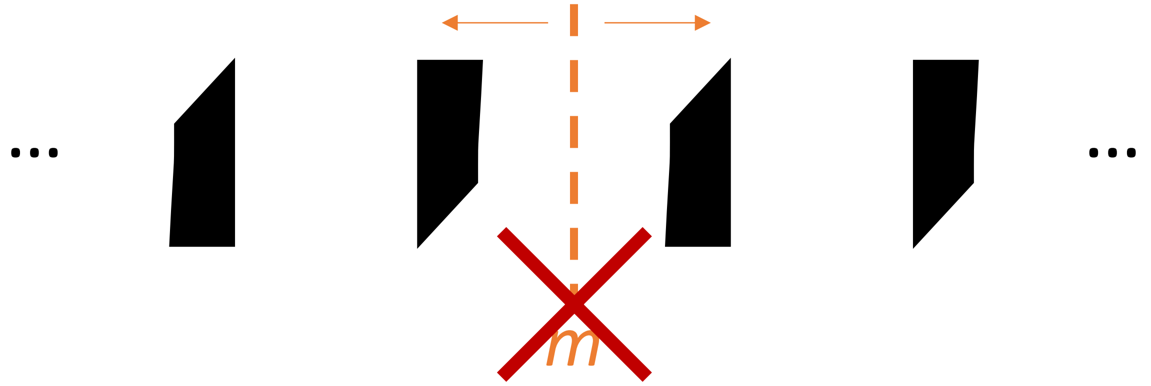
$\vec{T}$ is a "***translation***" symmetry operation

- Since the system is infinite, if the entire chain were shifted by this amount, you wouldn't be able to tell that anything had happened
- This is a defining feature of any symmetry operation

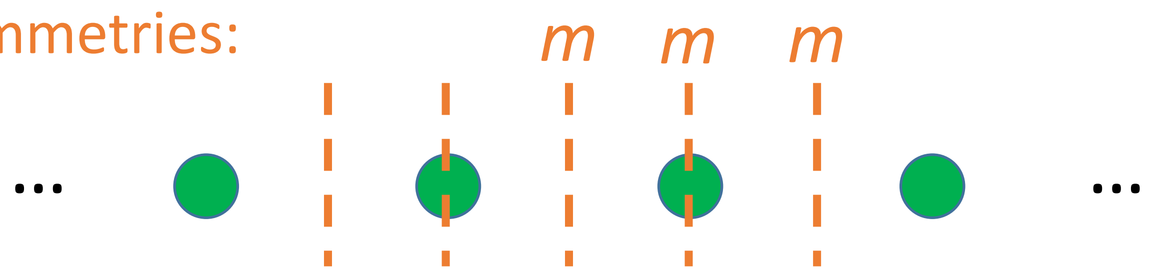
Symmetry

Another symmetry operation that is possible in 1D is ***mirror symmetry*, or *reflection*.**

Here there is no mirror symmetry due to the *chiral motifs.* This can be seen by trying to place a mirror any where:

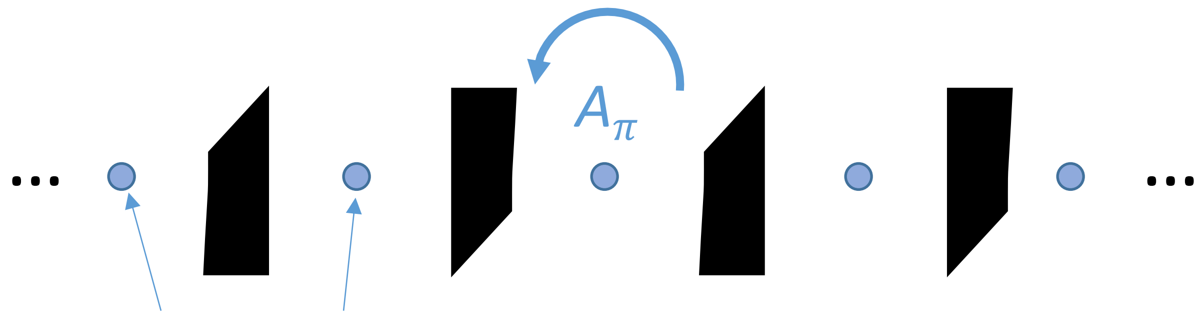


However, if the motifs were symmetric then we would have mirror symmetries:



Symmetry

If we allow the system to move in 2D, then we have an additional symmetry operation: ***rotation***. In 2D, rotation must be defined about a specific point (and in 3D, it must be defined about a specific axis).

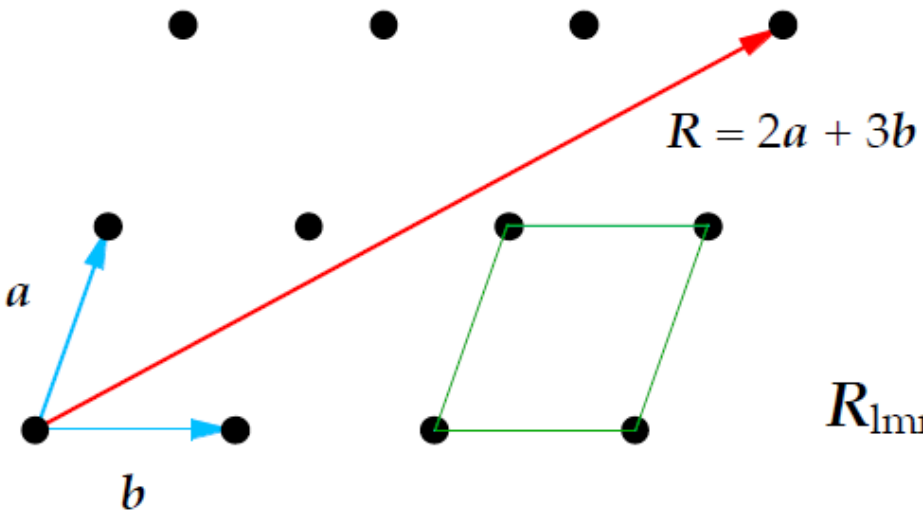


We could rotate the entire system by π radians (180°) about any of these points (but not elsewhere!).

These points could be indicated by writing A_π (to indicate rotation by π radians at point A) or, equivalently, by writing C_2 to indicate a "2-fold" rotation axis (we'll talk more about this later).

The 2D space lattice

- Every point in the space lattice is identical
- The translation vector tells how to get from any point to any other equivalent point



$$R_{\mathrm{lmn}} = \mathrm{l}\boldsymbol{a} + \mathrm{m}\boldsymbol{b} + \mathrm{n}\boldsymbol{c}$$

- $\boldsymbol{a}$, $\boldsymbol{b}$, $\boldsymbol{c}$ are lattice vectors; l, m, n are integers
- A good set of lattice vectors allows the translation vector to span from any point in the lattice to any other
- Unit cell is parallelepiped whose edges are $\boldsymbol{a}$, $\boldsymbol{b}$, $\boldsymbol{c}$

2D symmetry operations

Symmetry operations involve transformation of coordinates:

1. Translation

$$(x,\ y) \xrightarrow{\vec{T}} (x+a,\ y+b) \xrightarrow{\vec{T}} (x+2a,\ y+2b)$$

2. Mirror / reflection

   Need to define a “mirror axis” (in 2D) or “mirror plane” (in 3D)

   E.g., for a mirror axis parallel with the y-axis in 2D:

$$(x,\ y) \xrightarrow{M} (-x,\ y) \xrightarrow{M} (x,\ y)$$

M changes the sense of *one* coordinate

3. Rotation

   Need to define a point (in 2D) or axis (in 3D) around which rotation occurs. E.g., $\boldsymbol{A}_\pi$ rotates everything by π radians around point *A*.

Rotation can change the sense of *two* coordinates