SAND2008-1986C

How close are two grain boundaries
in the five dimensional crystallographic space?

David Olmsted

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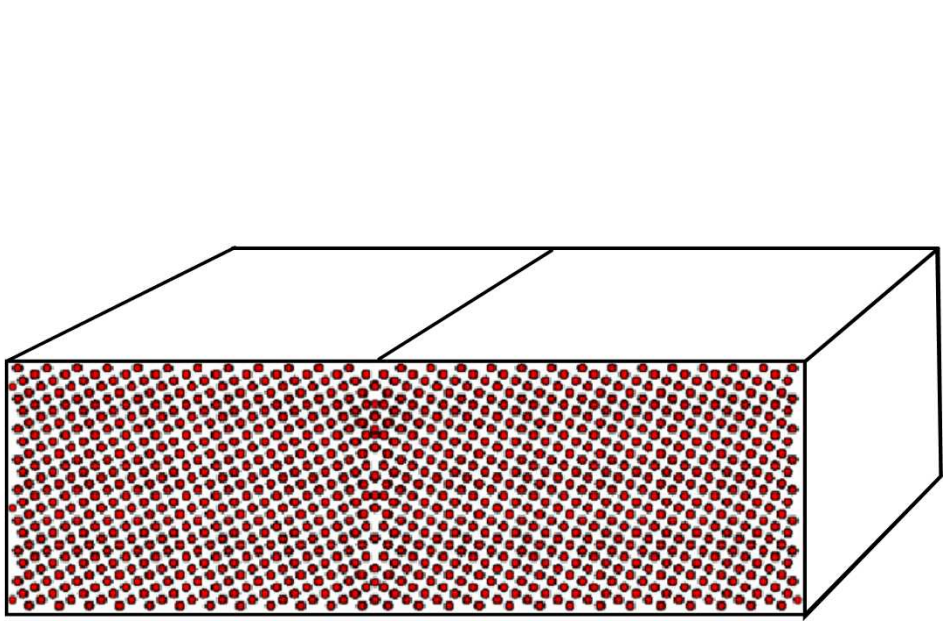

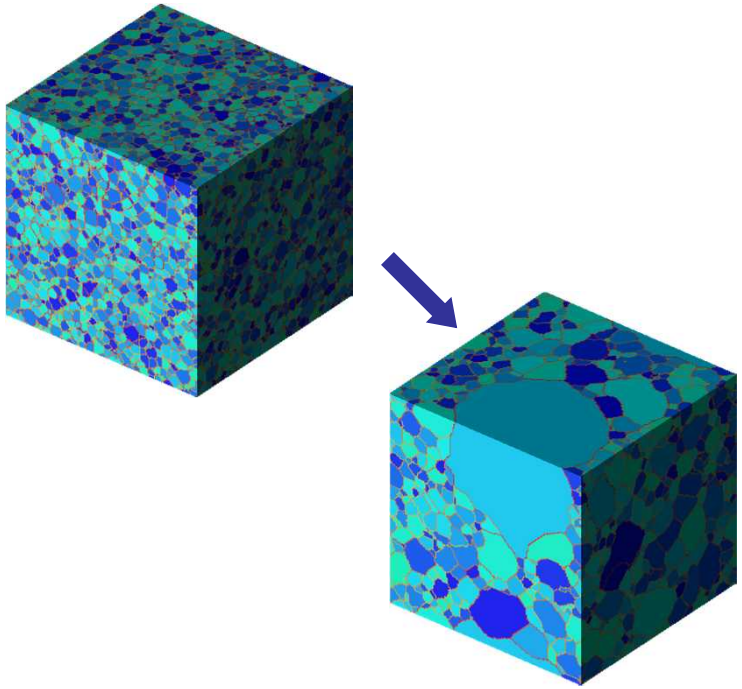

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Distance in 5d grain boundary space

- **Why**
- **Method**

  Describe single boundary in 5d space

  Define distance between two boundaries
- **Examples**

Other distances:

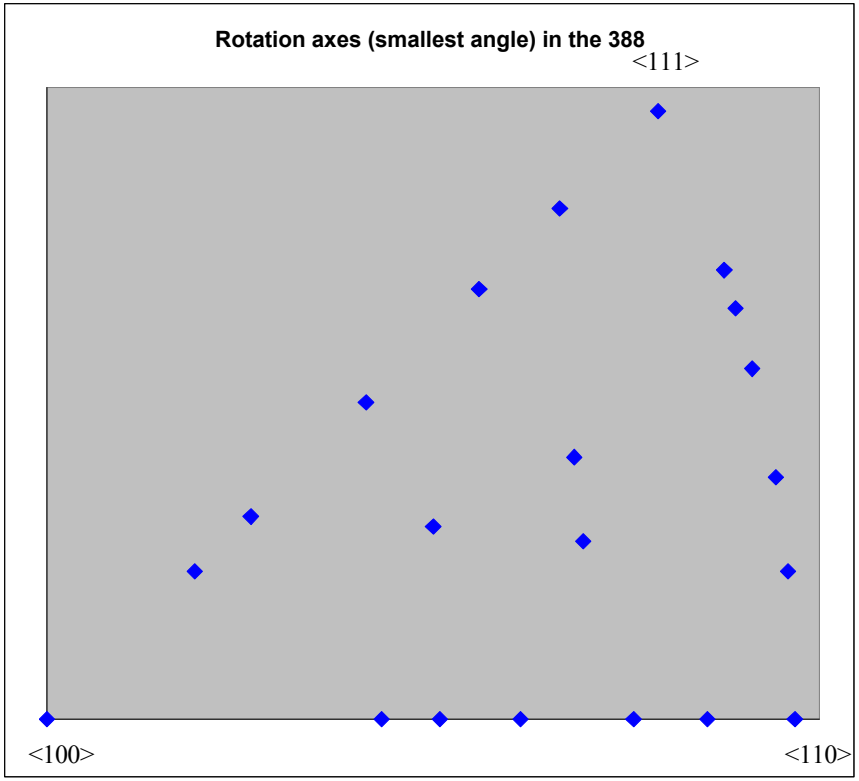
A. Moraweic, 1998

J.W. Cahn & J.E. Taylor, 2006

Need distance to interpolate

- For mesoscale simulations we need to assign properties to any boundary.
- To look up an arbitrary boundary in table, we need to find the most similar table boundary.
- Presumably this is the closest boundary in the 5d macroscopic grain boundary space.

Need distance to fill in table



Add optimal boundaries from larger set, not all.

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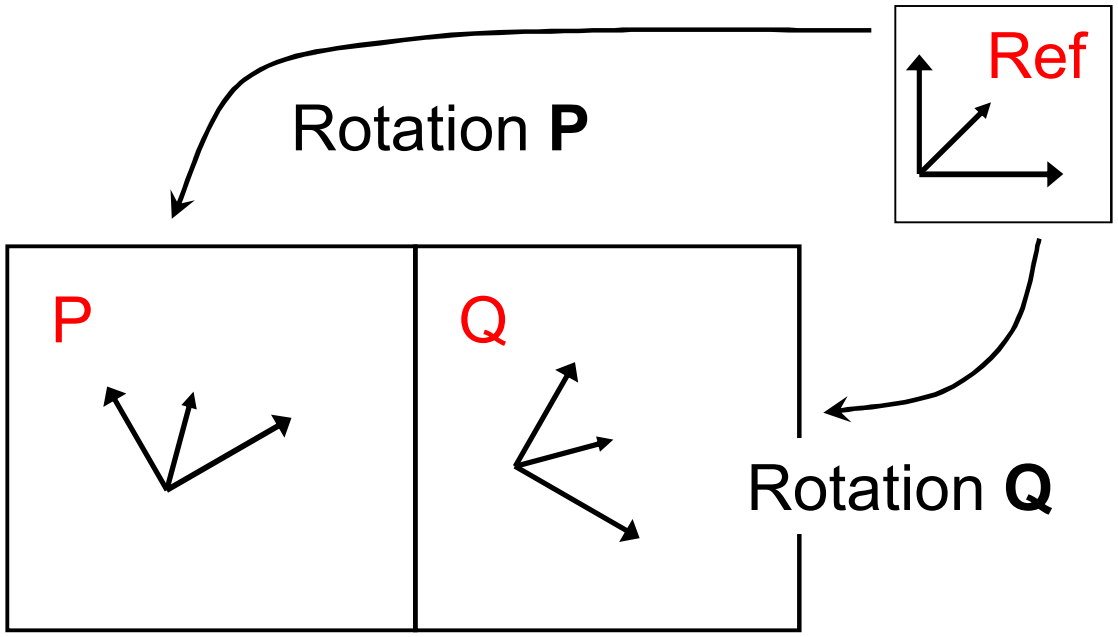
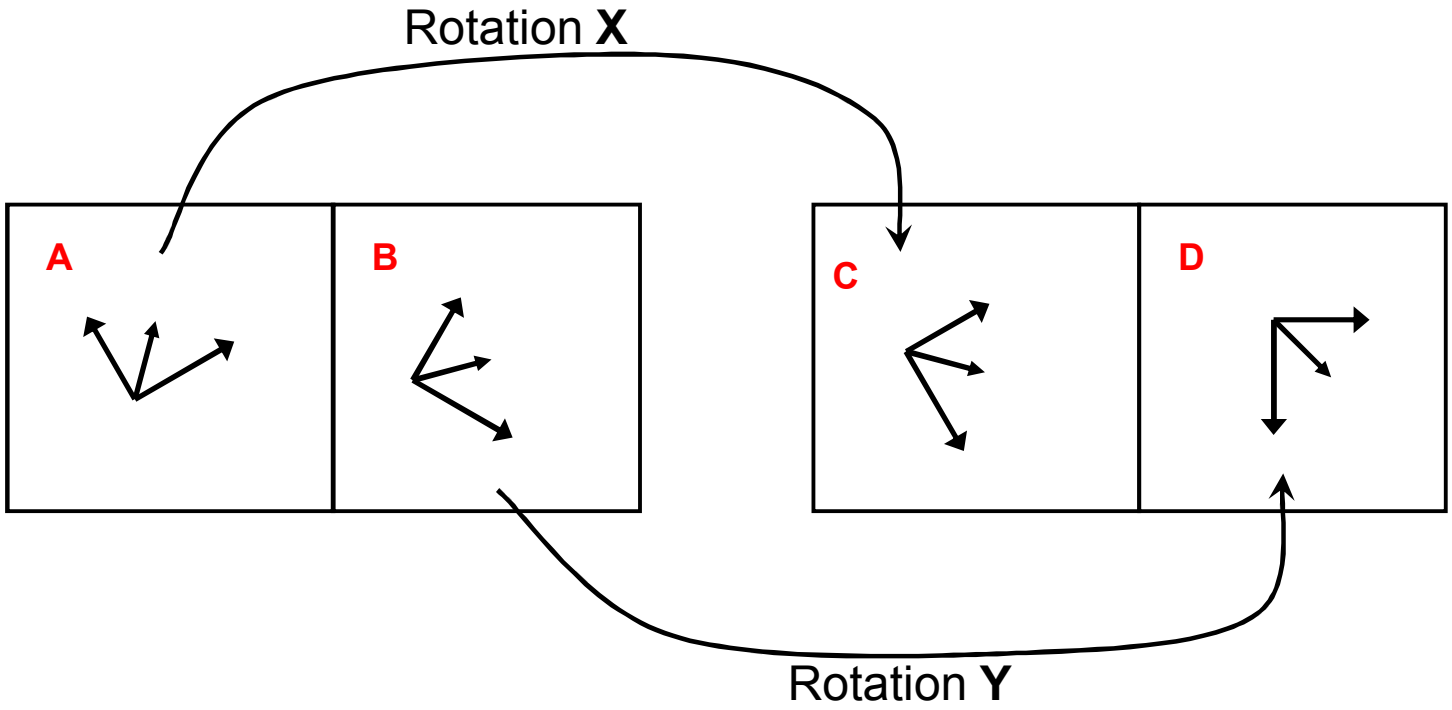
Describe position in 5d space



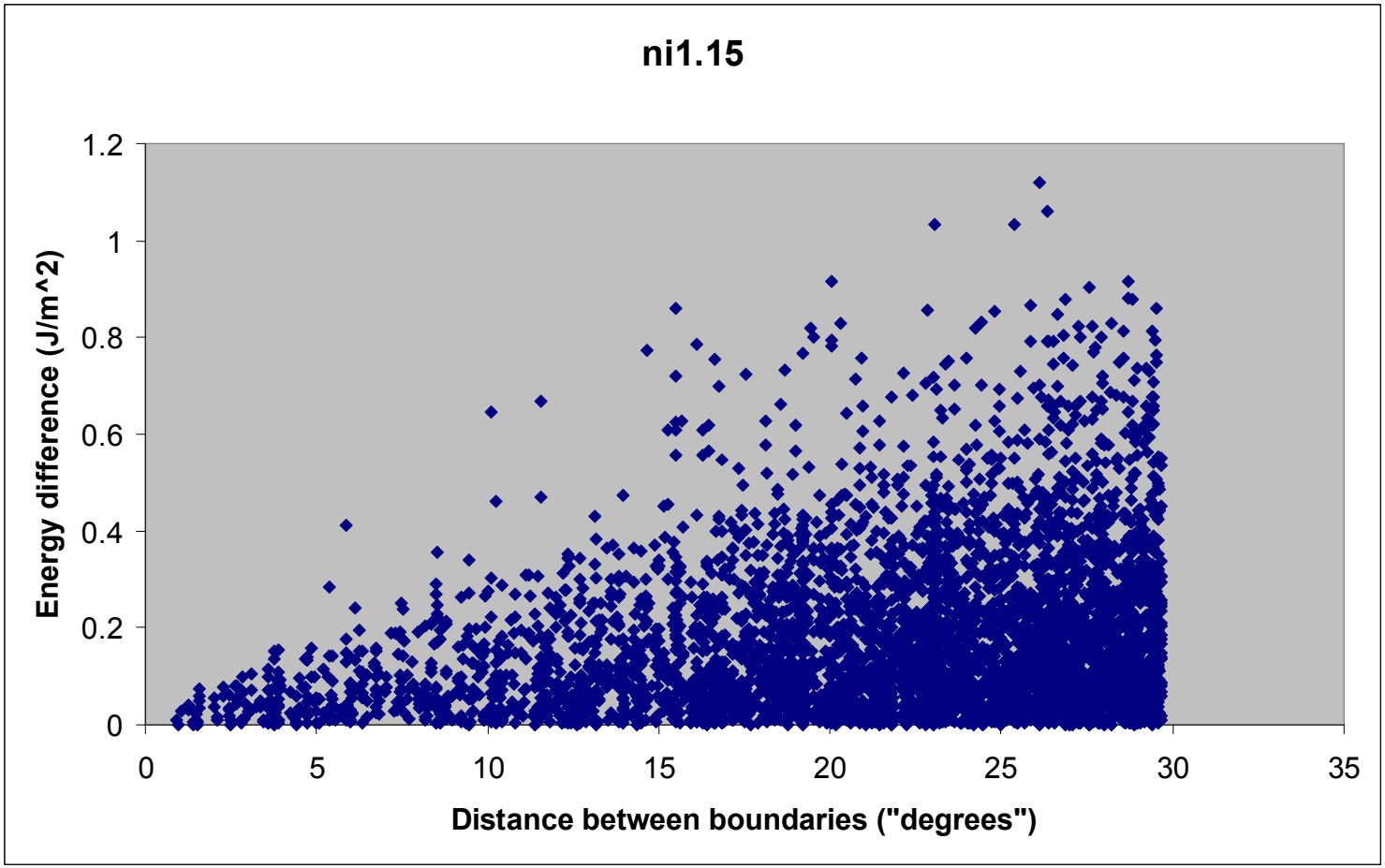
(**P**,**Q**) describes boundary, but we have to allow for fcc symmetries **and** rotations about boundary normal.

Distance between two boundaries



d(AB,CD)=|X|+|Y| minimized over all equivalent representations of boundaries AB and CD

Nearby boundaries have similar energy



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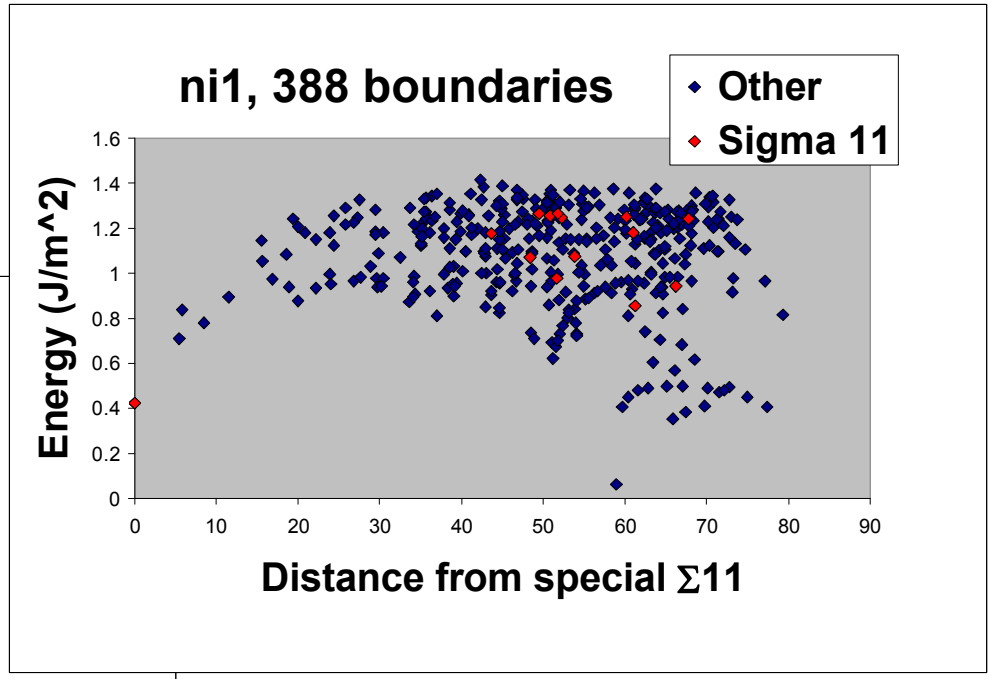
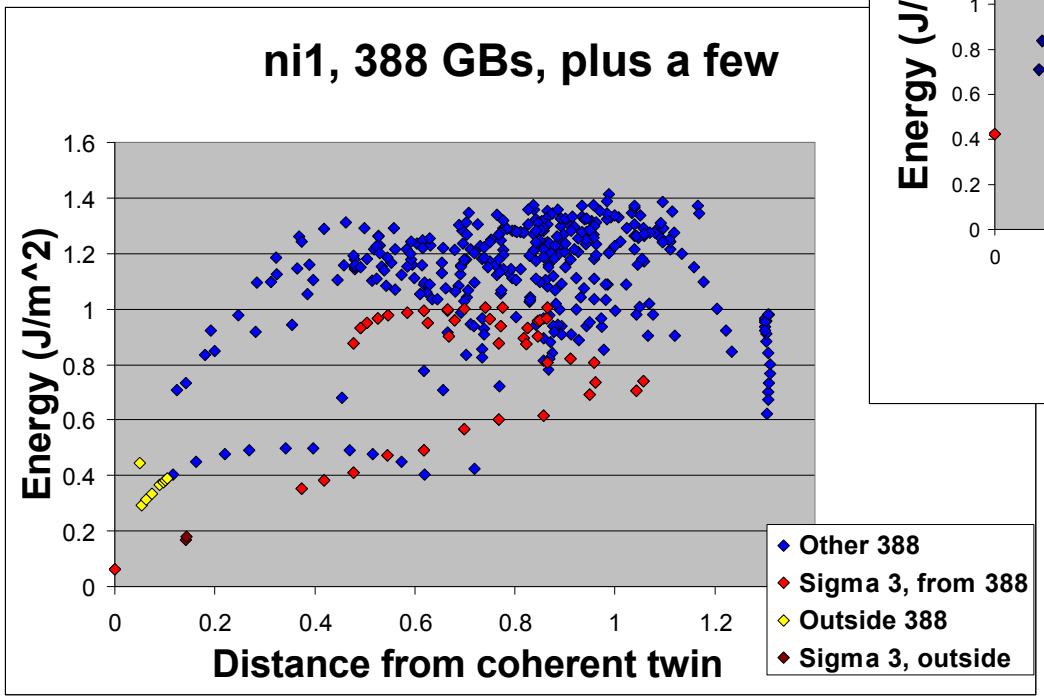
Energy cusps





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Distance in 5d grain boundary space

- A distance is needed to access table of “388” GBs for an arbitrary boundary.
- Distance is needed to fill in holes in the table.
- For the distance shown here, nearby boundaries have similar energy.
- Distance can also be used to examine, for example, the existence of energy cusps.