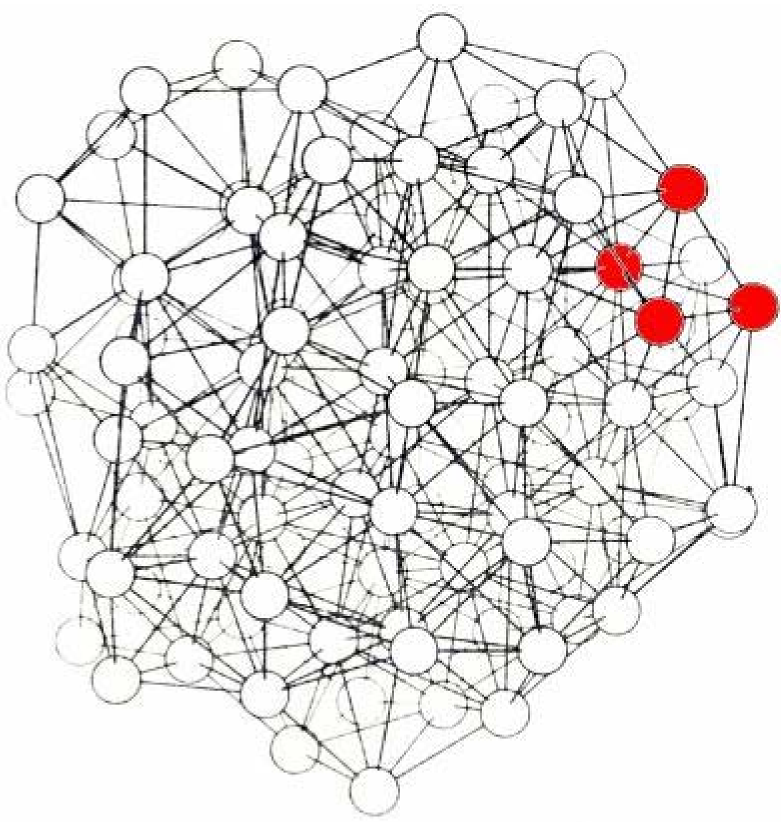
Tetrahedral motifs in amorphous systems



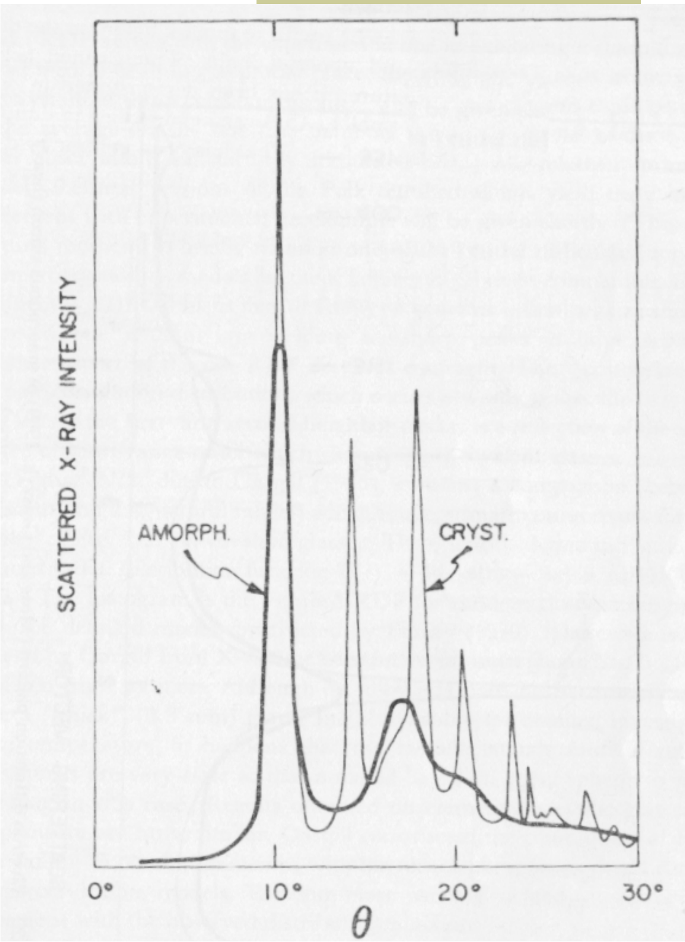
Matt Chambers

What is the short-range order of a liquid?

- Random?

Radial Distribution Function

- The nearest-neighbor distance disproves a complete lack of short-range order.



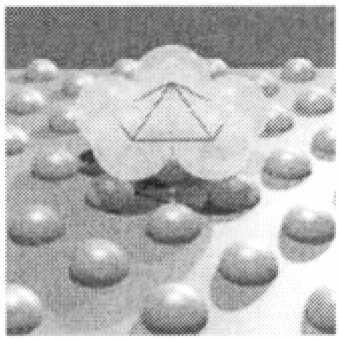
Zallen, Physics of Amorphous Solids, Wiley&Sons (1983)

What is the short-range order of a liquid?

- ~~Random?~~
- Micro-crystalline?

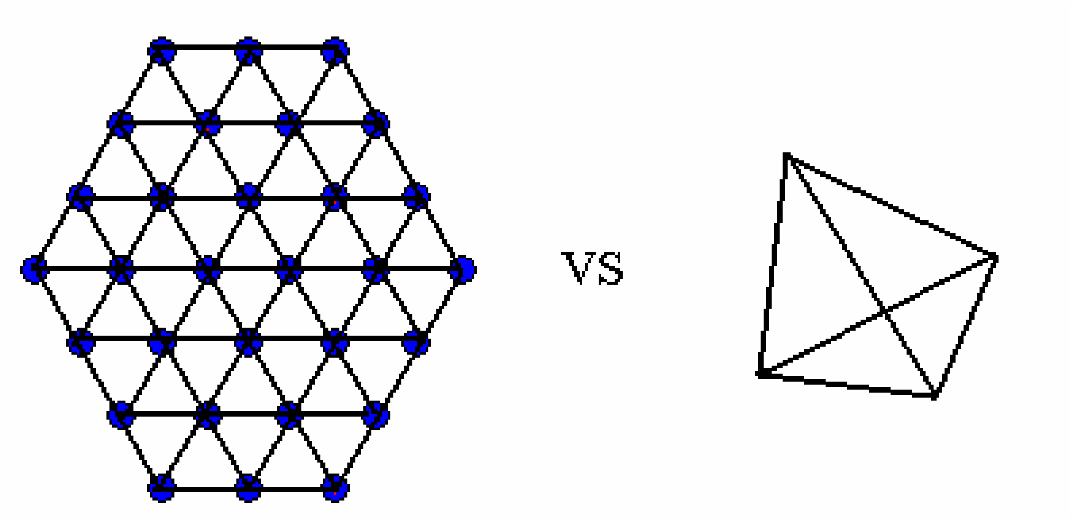
What is the short-range order of a liquid?

- ~~Random?~~
- ~~Micro-crystalline?~~
  - Disproved by Turnbull's mercury supercooling
- Quasicrystalline
- Icosahedral coordination shells are energetically more stable



Reichert, Nature **408** (2000) 839

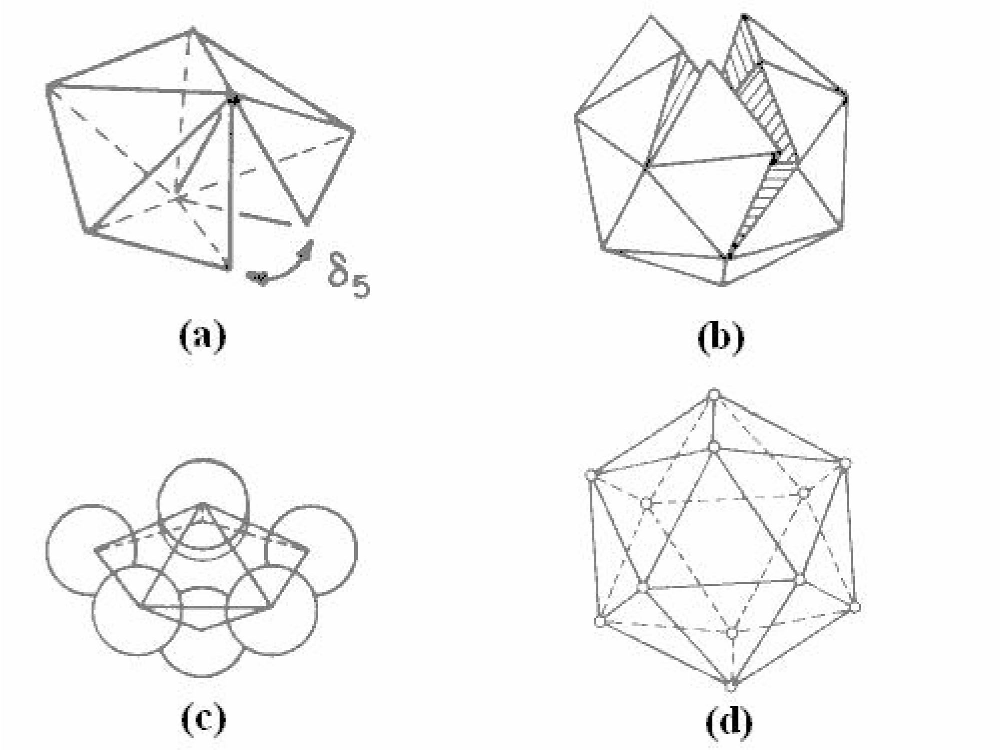
The Problem of Tiling Space



- A plane can be tiled with equilateral triangles
- Hard disc packing is ~90% efficient
- A single tetrahedron is ~78% packing efficiency
- However, perfect tetrahedra do not tile space

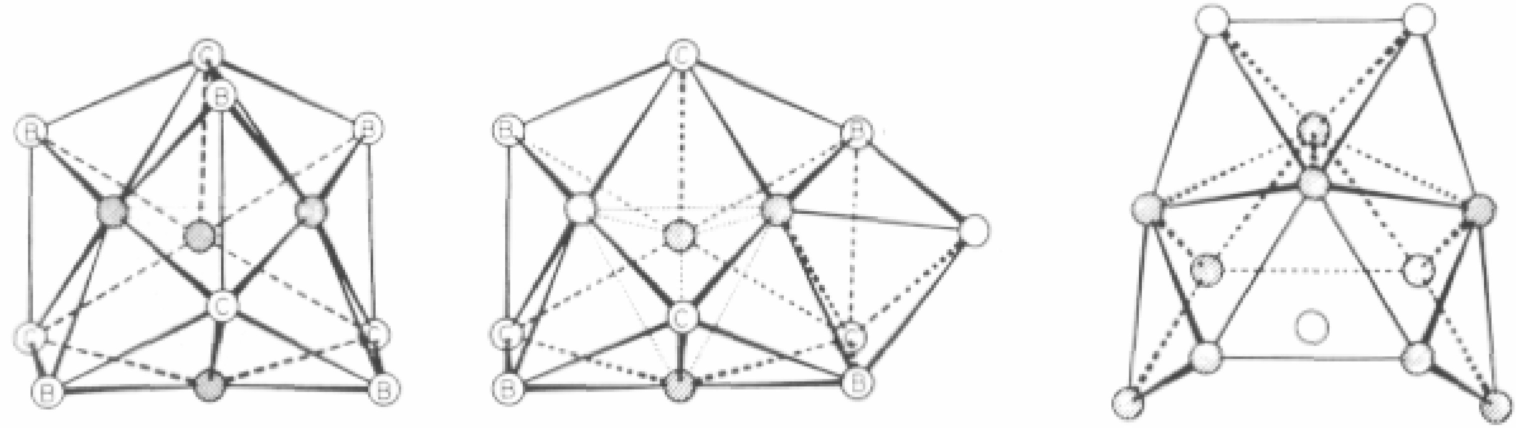
Assembling Tetrahedra

- Tetrahedra can *almost* assemble into pentagonal bipyramids or icosahedra
- A small distortion is needed to complete the regular polyhedron
- ~5% for icosahedra



Neslon and Spaepen, Solid State Phys. **42** (1989)

Stranger arrangements are possible



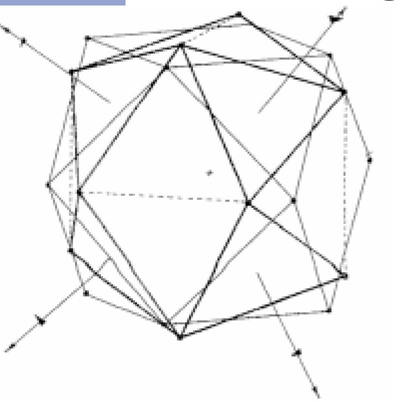
Neslon and Spaepen, Solid State Phys. **42** (1989)

Icosahedral Packing versus FCC, HCP, RCP

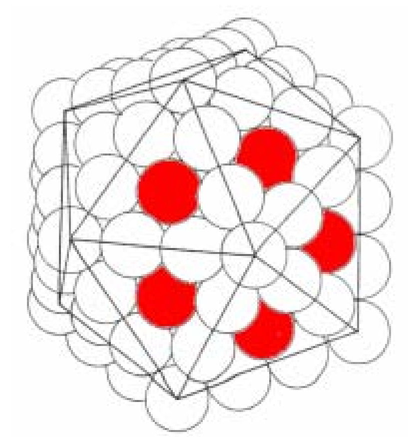
	Packing Efficiency	Fills Space	Coordination
Icosahedral Packing	0.726 to 0.681 depending on cluster size	No	Icosahedron
FCC Packing	0.740	Yes	Cube octahedron
HCP Packing	0.740, less if c/a>1	Yes	Twinned cube octahedron
Random Close Packing	0.637	Yes	Various

Transformations between cluster types

- Icosahedral clusters of 55 atoms or larger contain atoms with a mixture of arrangements.
- As clusters increase in size, the percentage of atoms with cube-octahedral coordination increases.
- The energy cost to change to *fcc* or *hcp* decreases with increasing cluster size.



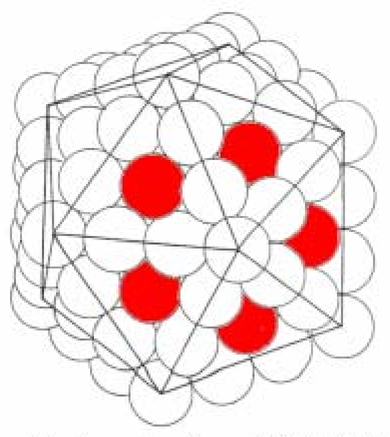
Mackay, Acta Cryst. **15**(1962) 916



Mackay, Acta Cryst. **15**(1962) 916

Problems scale with size

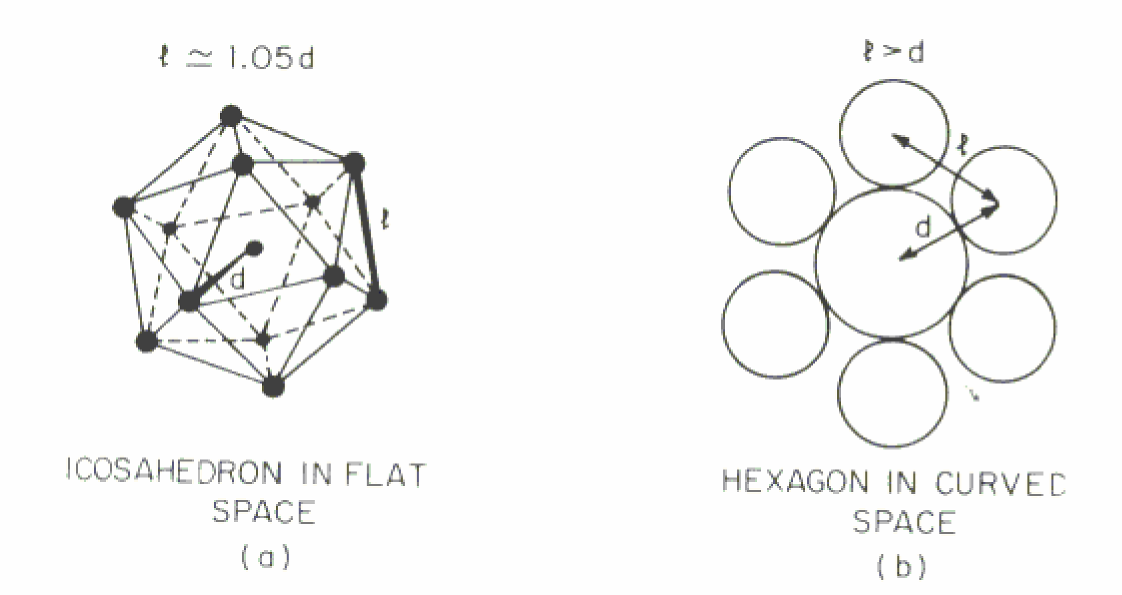
- Packing density of icosahedra decreases with size (to a minimum of 0.681)
- Icosahedra cannot tile space
- Large icosahedra contain many atoms with a cube-octahedron coordination shell



Mackay, Acta Cryst. **15**(1962) 916

Bent Space

- Tetrahedra can tile a space with appropriate curvature



Neslon and Spaepen, Solid State Phys. **42** (1989)

Modified Icosahedra: Frank-Kasper Polyhedra

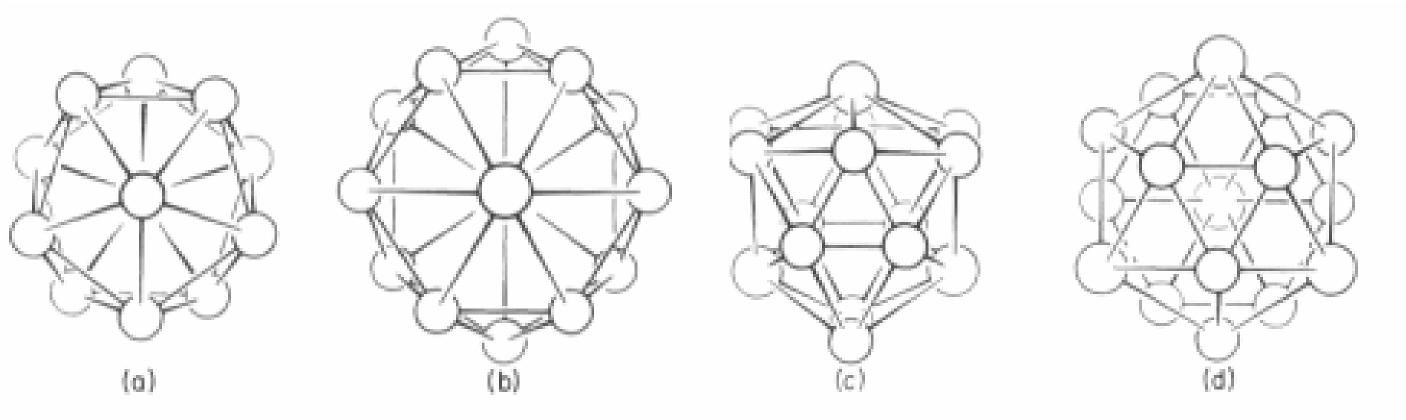
- The statistical honeycomb model predicts a coordination of 13.4[1]
- Additional atoms can be added to icosahedra as defects
- Added atoms must be added such that[2]:
  - The polyhedra remains triangulated
  - They are either S_5 or S_6

1 Neslon and Spaepen, Solid State Phys. **42** (1989)

2 Frank, Kasper, Acta Cryst. **11** (1958), 184

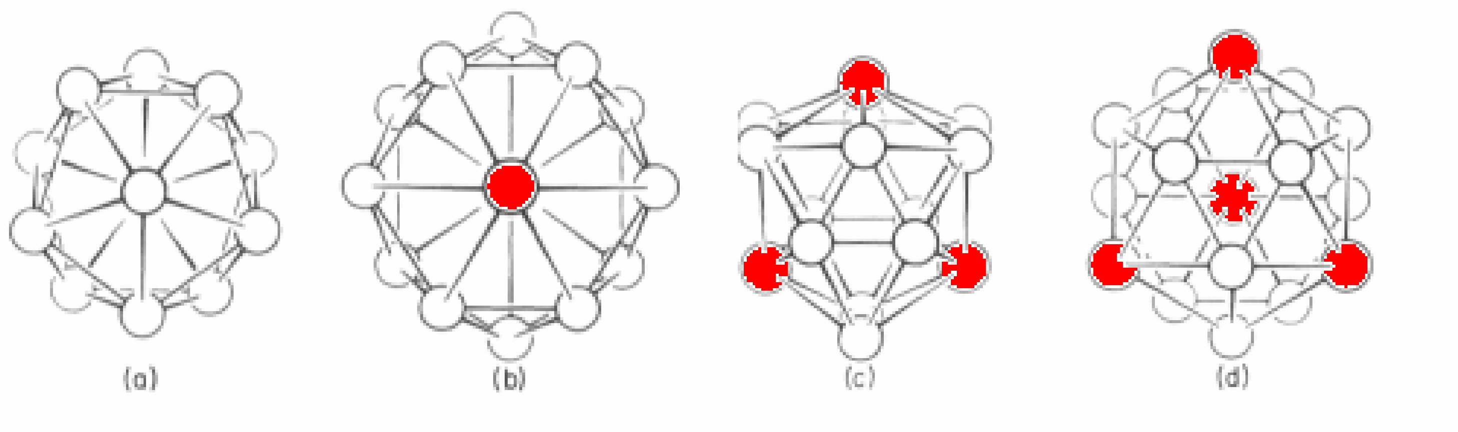
Modified Icosahedra: Frank-Kasper Polyhedra

- The regular icosahedra is referred to as Z12
- Z14, Z15, and Z16 polyhedra are also possible
- Z13 cannot be made triangulated



Modified Icosahedra: Frank-Kasper Polyhedra

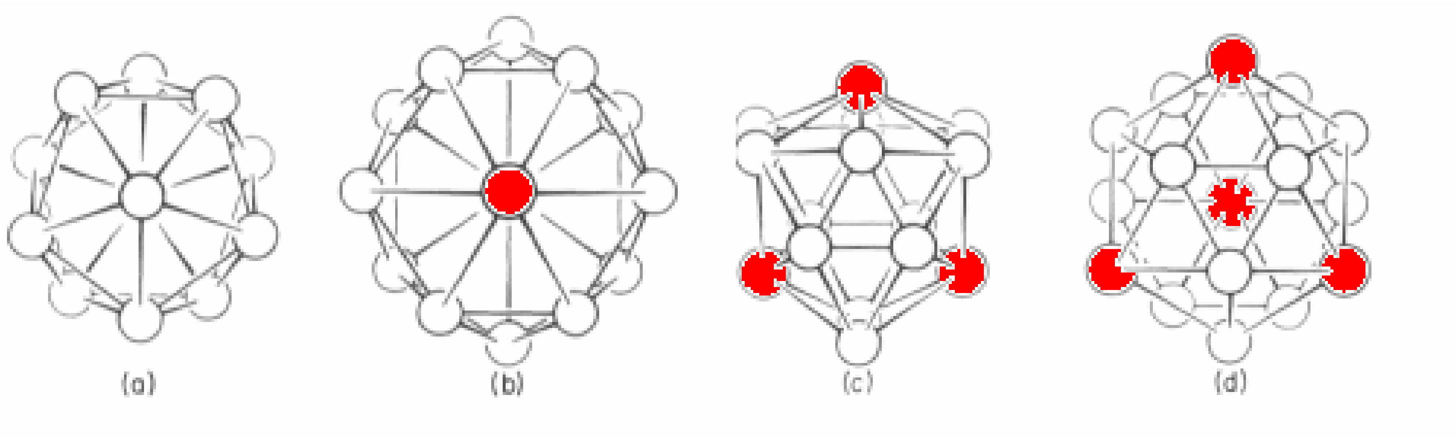
- Each polyhedra is unique
- The arrangement of S_6 atoms in each is precise.



(a) (b) (c) (d)

Tiling Space

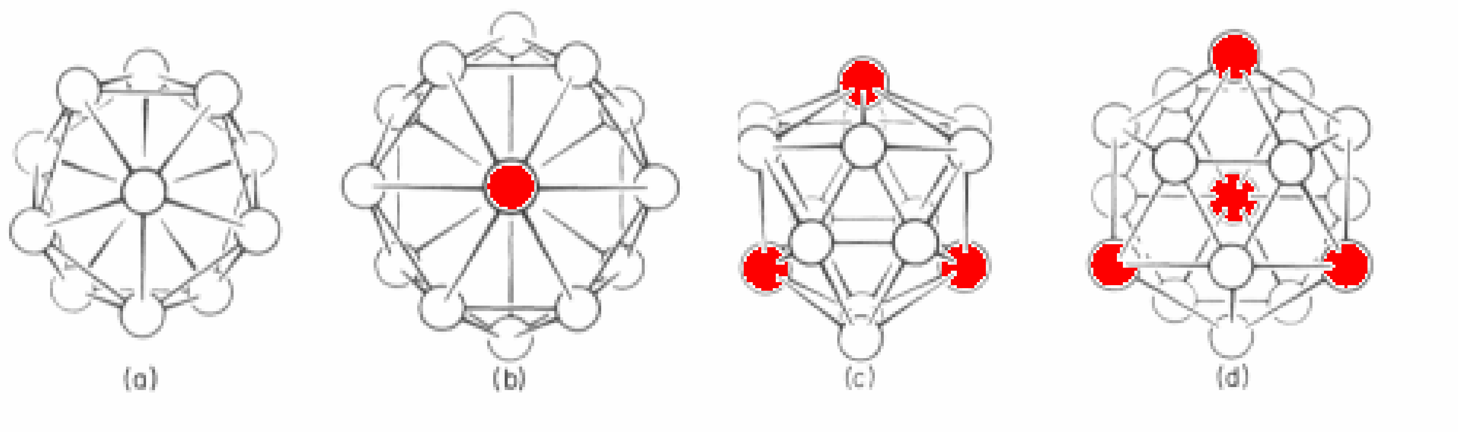
- Frank-Kasper polyhedra can tile space[3]
- A mixture of Z12 polyhedra with any of Z14, Z15 and Z16 is sufficient



3. Nelson, Phys. Rev. Let. **50** (1983), 982

Disclinations

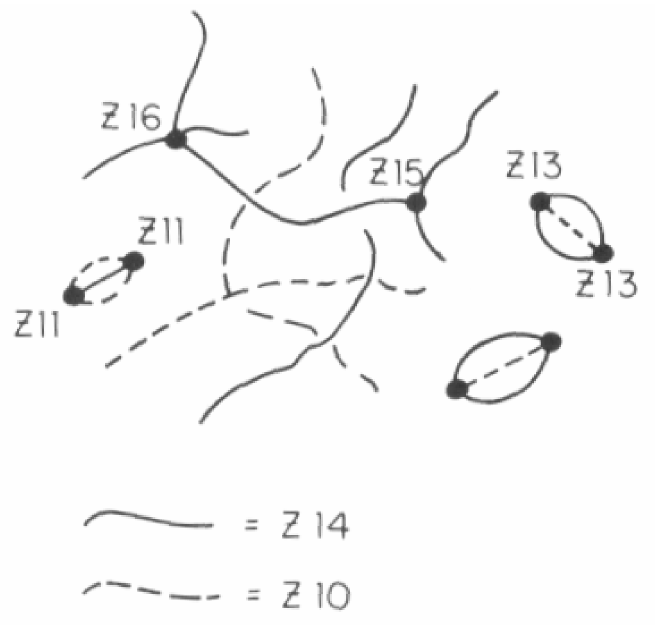
- Each S_6 atom must be shared by at least two polyhedra
- Connecting S_6 atoms shared by polyhedra leads to a network
- The network extends throughout the structure
- For Z14, Z15, and Z16, these are negative



4 Doye and Wales, Phys. Rev. Let. **86** (2000) 5719

Disclination Networks

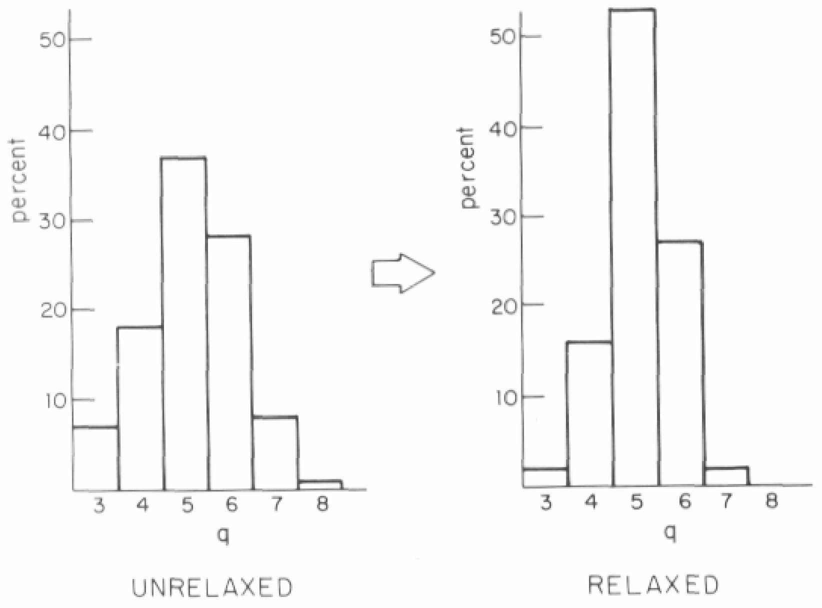
- Z8, Z9, and Z10 polyhedra are also possible, which produce positive disclinations.
- Geometry of positive disclinations is similar to negative disclinations (albeit with S_4 atoms).
- Disclinations interact with each other, including entanglement and annihilation interactions.



Nelson, Phys. Rev. Lett. **50** (1983), 982

More about disclinations

- Positive disclinations dominate (recall that the statistical coordination was 13.4)
- Ordered close-packed alloys can be described in terms of ordered disclinations
- Amorphous alloys contain disordered disclinations



Neslon and Spaepen, Solid State Phys. **42** (1989)