STRUTTURA DEI VETRI

THE ATOMIC ARRANGEMENT IN GLASS

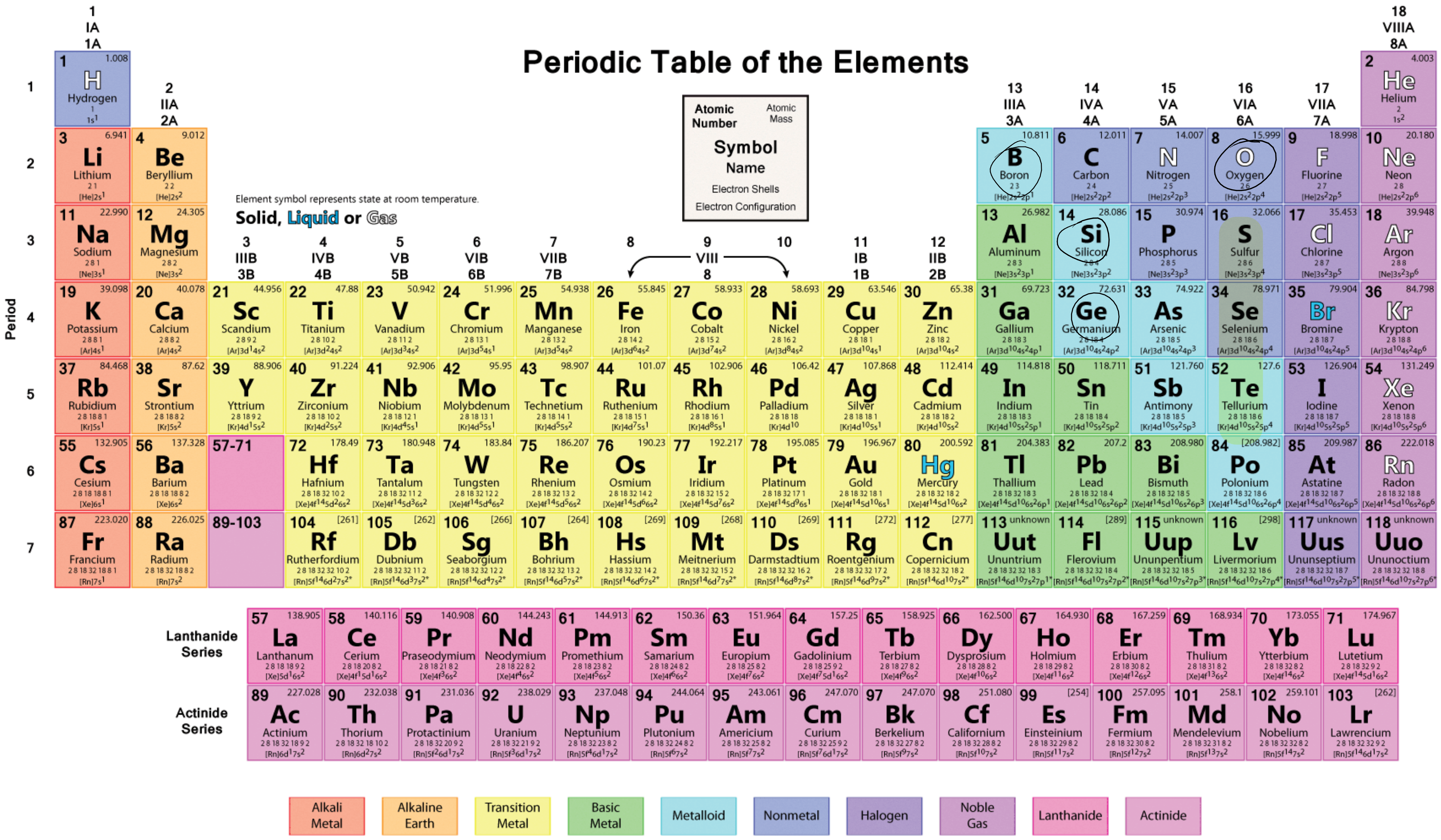
By W. H. Zachariasen

Received May 13, 1932 Published October 5, 1932

1. Introduction

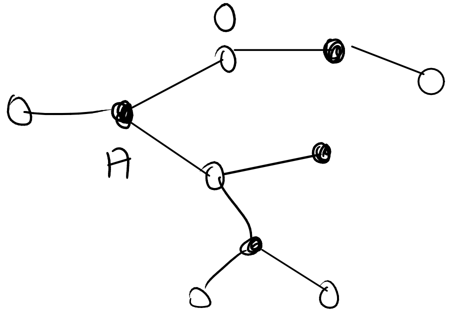
It must be frankly admitted that we know practically nothing about the atomic arrangement in glasses. Glasses are described as supercooled liquids or as solids. The former term is justifiable from the point of view of physical chemistry, the latter from the theory of elasticity. It seems rather futile, however, to try to decide which of the two descriptions is the proper one to use, when we are ignorant about the characteristic properties of the atomic arrangement.

- network-forming systems (SiO_2, GeO_2, B_2O_3) → continuous random network
- close-packed systems (metalli, colloidi, polimeri) → random close packing
- frustrazione geometrica → struttura localmente preferita


Periodic Table of the Elements
Atomic Number
Atomic Mass
Symbol
Name
Electron Shells
Electron Configuration
Element symbol represents state at room temperature.
Solid, Liquid or Gas
Period
1 IA 1A
2 IIA 2A
3 IIIB 3B
4 IVB 4B
5 VB 5B
6 VIB 6B
7 VIIB 7B
8
9 VIII 8
10
11 IB 1B
12 IIB 2B
13 IIIA 3A
14 IVA 4A
15 VA 5A
16 VIA 6A
17 VIIA 7A
18 VIIIA 8A
1 H Hydrogen 1.008
2 He Helium 4.003
3 Li Lithium 6.941
4 Be Beryllium 9.012
5 B Boron 10.811
6 C Carbon 12.011
7 N Nitrogen 14.007
8 O Oxygen 15.999
9 F Fluorine 18.998
10 Ne Neon 20.180
11 Na Sodium 22.990
12 Mg Magnesium 24.305
13 Al Aluminum 26.982
14 Si Silicon 28.086
15 P Phosphorus 30.974
16 S Sulfur 32.066
17 Cl Chlorine 35.453
18 Ar Argon 39.948
19 K Potassium 39.098
20 Ca Calcium 40.078
21 Sc Scandium 44.956
22 Ti Titanium 47.88
23 V Vanadium 50.942
24 Cr Chromium 51.996
25 Mn Manganese 54.938
26 Fe Iron 55.845
27 Co Cobalt 58.933
28 Ni Nickel 58.693
29 Cu Copper 63.546
30 Zn Zinc 65.38
31 Ga Gallium 69.723
32 Ge Germanium 72.631
33 As Arsenic 74.922
34 Se Selenium 78.971
35 Br Bromine 79.904
36 Kr Krypton 84.798
37 Rb Rubidium 84.468
38 Sr Strontium 87.62
39 Y Yttrium 88.906
40 Zr Zirconium 91.224
41 Nb Niobium 92.906
42 Mo Molybdenum 95.95
43 Tc Technetium 98.907
44 Ru Ruthenium 101.07
45 Rh Rhodium 102.906
46 Pd Palladium 106.42
47 Ag Silver 107.868
48 Cd Cadmium 112.414
49 In Indium 114.818
50 Sn Tin 118.711
51 Sb Antimony 121.760
52 Te Tellurium 127.6
53 I Iodine 126.904
54 Xe Xenon 131.249
55 Cs Cesium 132.905
56 Ba Barium 137.328
57-71
72 Hf Hafnium 178.49
73 Ta Tantalum 180.948
74 W Tungsten 183.84
75 Re Rhenium 186.207
76 Os Osmium 190.23
77 Ir Iridium 192.217
78 Pt Platinum 195.085
79 Au Gold 196.967
80 Hg Mercury 200.592
81 Tl Thallium 204.383
82 Pb Lead 207.2
83 Bi Bismuth 208.980
84 Po Polonium [208.982]
85 At Astatine 209.987
86 Rn Radon 222.018
87 Fr Francium 223.020
88 Ra Radium 226.025
89-103
104 Rf Rutherfordium [261]
105 Db Dubnium [262]
106 Sg Seaborgium [266]
107 Bh Bohrium [264]
108 Hs Hassium [269]
109 Mt Meitnerium [268]
110 Ds Darmstadtium [269]
111 Rg Roentgenium [272]
112 Cn Copernicium [277]
113 Uut Ununtrium unknown
114 Fl Flerovium [289]
115 Uup Ununpentium unknown
116 Lv Livermorium [298]
117 Uus Ununseptium unknown
118 Uuo Ununoctium unknown
Lanthanide Series
57 La Lanthanum 138.905
58 Ce Cerium 140.116
59 Pr Praseodymium 140.908
60 Nd Neodymium 144.243
61 Pm Promethium 144.913
62 Sm Samarium 150.36
63 Eu Europium 151.964
64 Gd Gadolinium 157.25
65 Tb Terbium 158.925
66 Dy Dysprosium 162.500
67 Ho Holmium 164.930
68 Er Erbium 167.259
69 Tm Thulium 168.934
70 Yb Ytterbium 173.055
71 Lu Lutetium 174.967
Actinide Series
89 Ac Actinium 227.028
90 Th Thorium 232.038
91 Pa Protactinium 231.036
92 U Uranium 238.029
93 Np Neptunium 237.048
94 Pu Plutonium 244.064
95 Am Americium 243.061
96 Cm Curium 247.070
97 Bk Berkelium 247.070
98 Cf Californium 251.080
99 Es Einsteinium [254]
100 Fm Fermium 257.095
101 Md Mendelevium 258.1
102 No Nobelium 259.101
103 Lr Lawrencium [262]
Alkali Metal
Alkaline Earth
Transition Metal
Basic Metal
Metalloid
Nonmetal
Halogen
Noble Gas
Lanthanide
Actinide

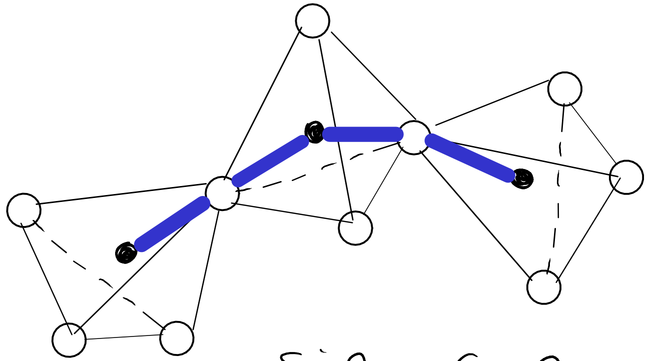
Network-forming glasses

1932 Zachariasen → $A_n O_m$



$\begin{cases} x_O \\ x_A \end{cases}$ concentrazioni $1 = x_A + x_O$

$\begin{cases} z_O \\ z_A \end{cases}$ n. coordinazione



SiO_2, GeO_2

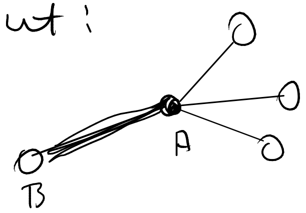
ES: z_A, z_B fissati

x_A, $x_B = 1 - x_A$ tali

che network connesso?

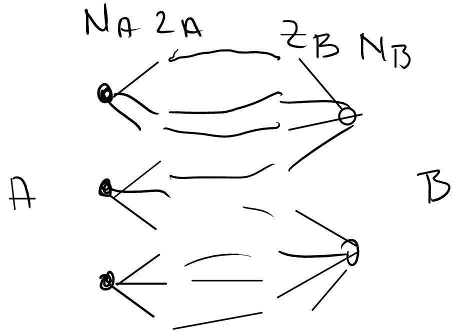
$$x_A z_A = x_B z_B$$

Hint:



$N_b \frac{1}{z_A} = N_B$

$N_b \frac{1}{z_B} = N_A$



$z_{Si} = 4$, $z_O = 2$

$4 x_{Si} = (1 - x_{Si})\, 2 \rightarrow 6 x_{Si} = 2 \rightarrow x_{Si} = 1/3 \rightarrow x_O = 2/3$

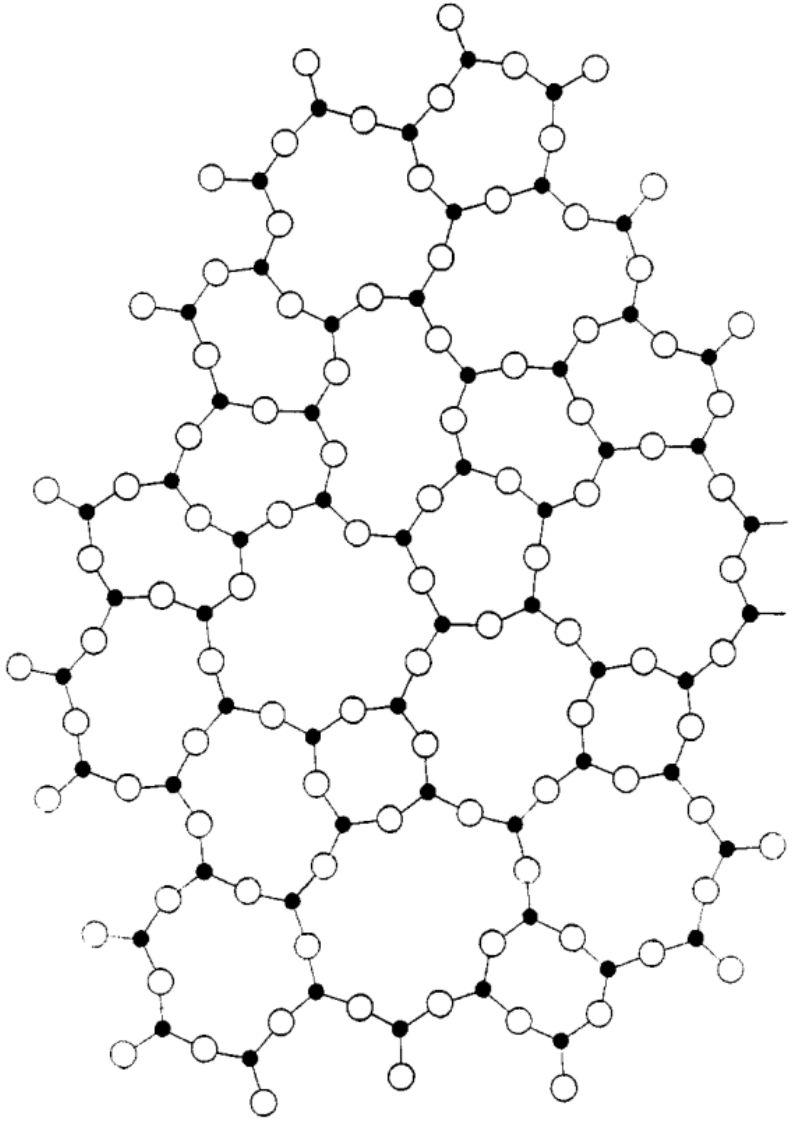


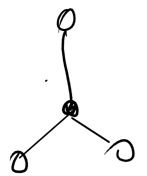
Fig. 1b.

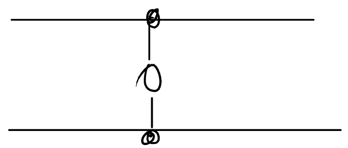
Zachariasen 1932

ES: Ge + Se

As + Se

Silice 2d ⇒ $x_{Si} = ?$ $x_O = ?$



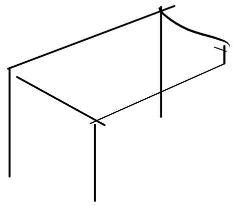


$$\begin{cases} z_{Si} = 3 \\ z_O = 2 \end{cases}$$

Teoria della rigidità

1) Gupta – Cooper (1978) ~ Zachariasen
2) Phillips – Thorpe (1979) → bonds

Idea: rigidità "minimale" → glass-forming ability
ISOSTATICITÀ



$n = 2$ instabile
$n = 3$ stabile marginale / isostaticità
$n = 4$ stabile

Criterio di Maxwell: isostaticità se

n. gradi libertà = n. vincoli

Direct Imaging of a Two-Dimensional Silica Glass on Graphene

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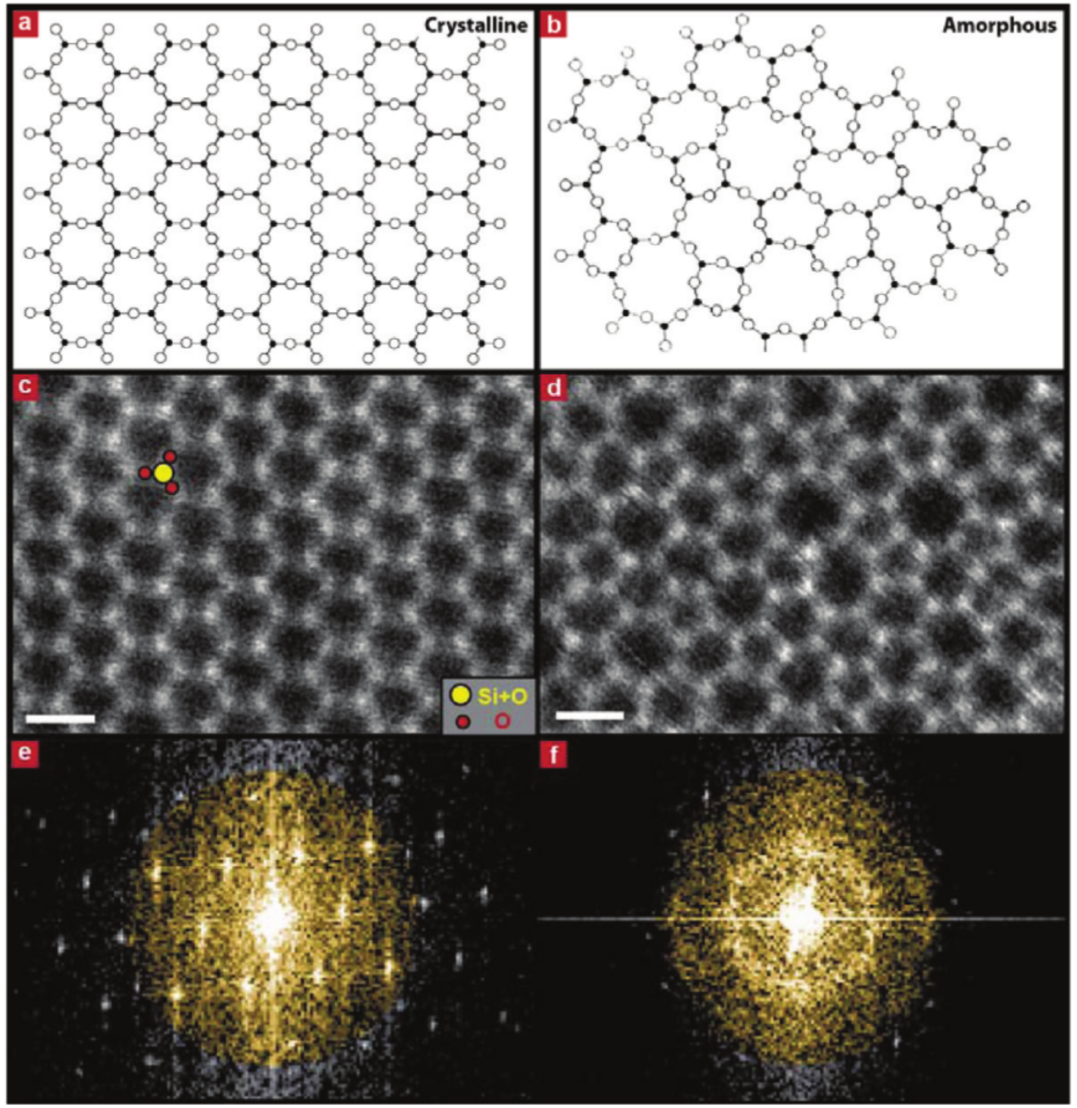
Nano Lett. 2012, 12, 1081–1086



T=0 fisso distanza legame + angoli tra 2 legami $z_\alpha \to$ legami specie α

$$N_v = \sum_\alpha N_\alpha \frac{z_\alpha}{2} + N_\alpha (2z_\alpha - 3) \to n_v = \sum_\alpha x_\alpha \left(\frac{z_\alpha}{2} + 2z_\alpha - 3 \right)$$

$$\langle z \rangle = \sum_\alpha x_\alpha z_\alpha \qquad n_v = \frac{\langle z \rangle}{2} + 2\langle z \rangle - 3$$

Condizione Maxwell $N \to \infty$

$$3N = N n_v + 6 \approx N n_v \Rightarrow n_v = 3 \quad (3d)$$

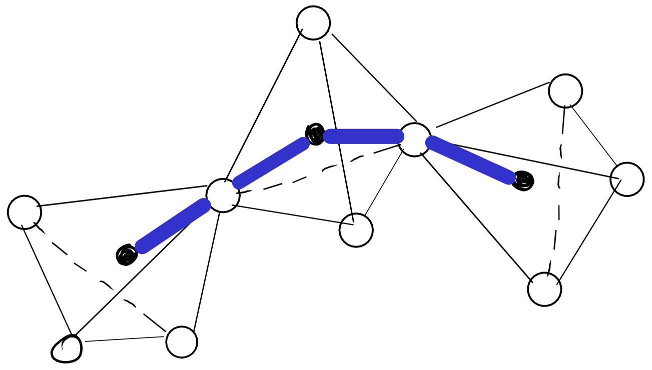
$$\frac{\langle z \rangle}{2} + 2\langle z \rangle = 6$$

$$\frac{5}{2}\langle z \rangle = 6$$

$$\langle z \rangle = \frac{12}{5} = 2.4 \quad (MF) \to SiO_2, GeO_2$$

Es: SiO_2

$$\langle z \rangle = \frac{1}{3} 4 + \frac{2}{3} 2 = \frac{8}{3} \gtrsim 2.4$$



Close-packed glasses

SUPERCOOLING OF LIQUIDS 1952

BY F. C. FRANK

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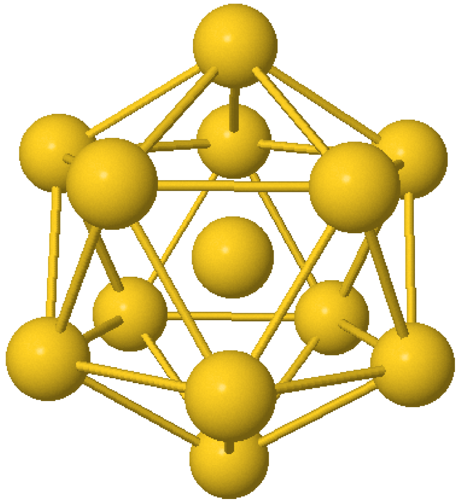
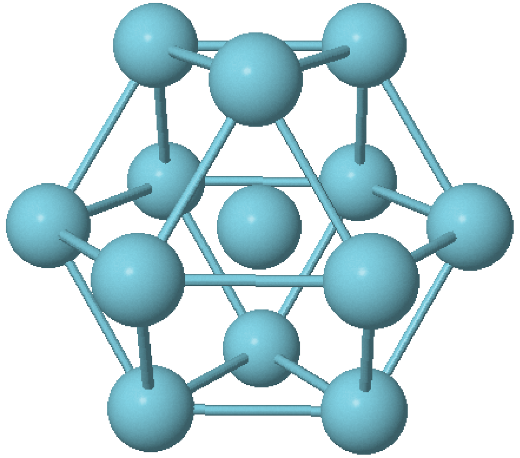
I shall concentrate upon reviewing the important recent change in our appreciation of the facts of supercooling which has been brought about particularly by the work of Turnbull at the General Electric Research Laboratory in Schenectady. I suppose that most of us, talking about supercooling a couple of years ago, would have divided substances into two classes, one with simple crystal structures like gold, and all the other 'good' metals on the one hand, and those with complex crystal structures, such as glycerol and the silicates on the other; saying that whereas the latter class can be very much supercooled, and will form glasses, the former class can only be supercooled a very few degrees. Then we would have added that there are some 'bad' metals, with moderately complex crystal structures, such as antimony or bismuth, which can be supercooled some tens of degrees, forming an intermediate class.

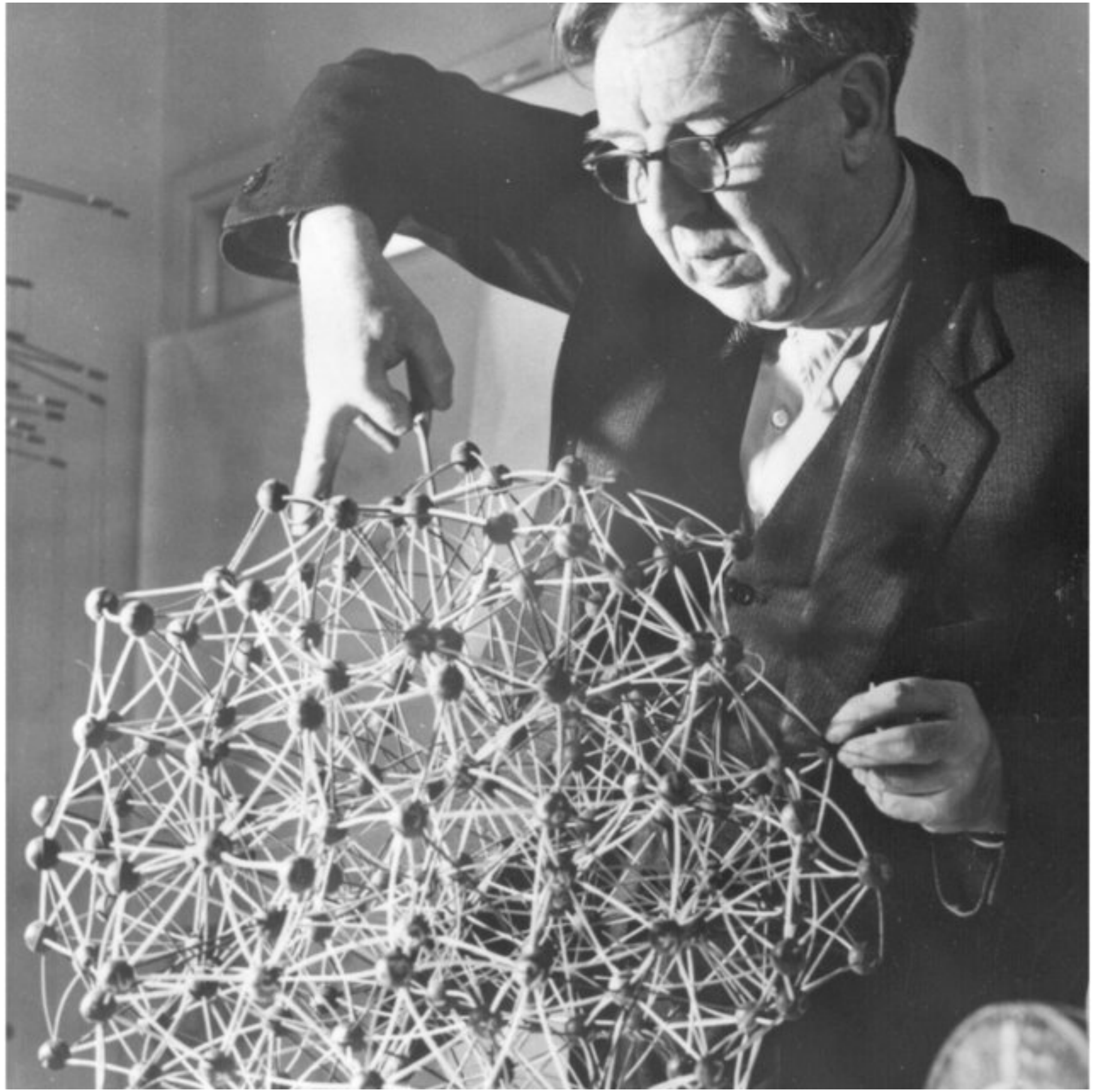


icosaedro



Fcc

→ frustrazione geometrica



Bernal 1964

Tassellazione di Voronoi

→ Wigner-Seitz

cella 3d ≡ poliedro

f : n. facce di un poliedro

p : n. vertici di ogni faccia

$$\bar{f} = \frac{12}{6 - \bar{p}}$$

$(f_3, f_4, f_5, \dots)$

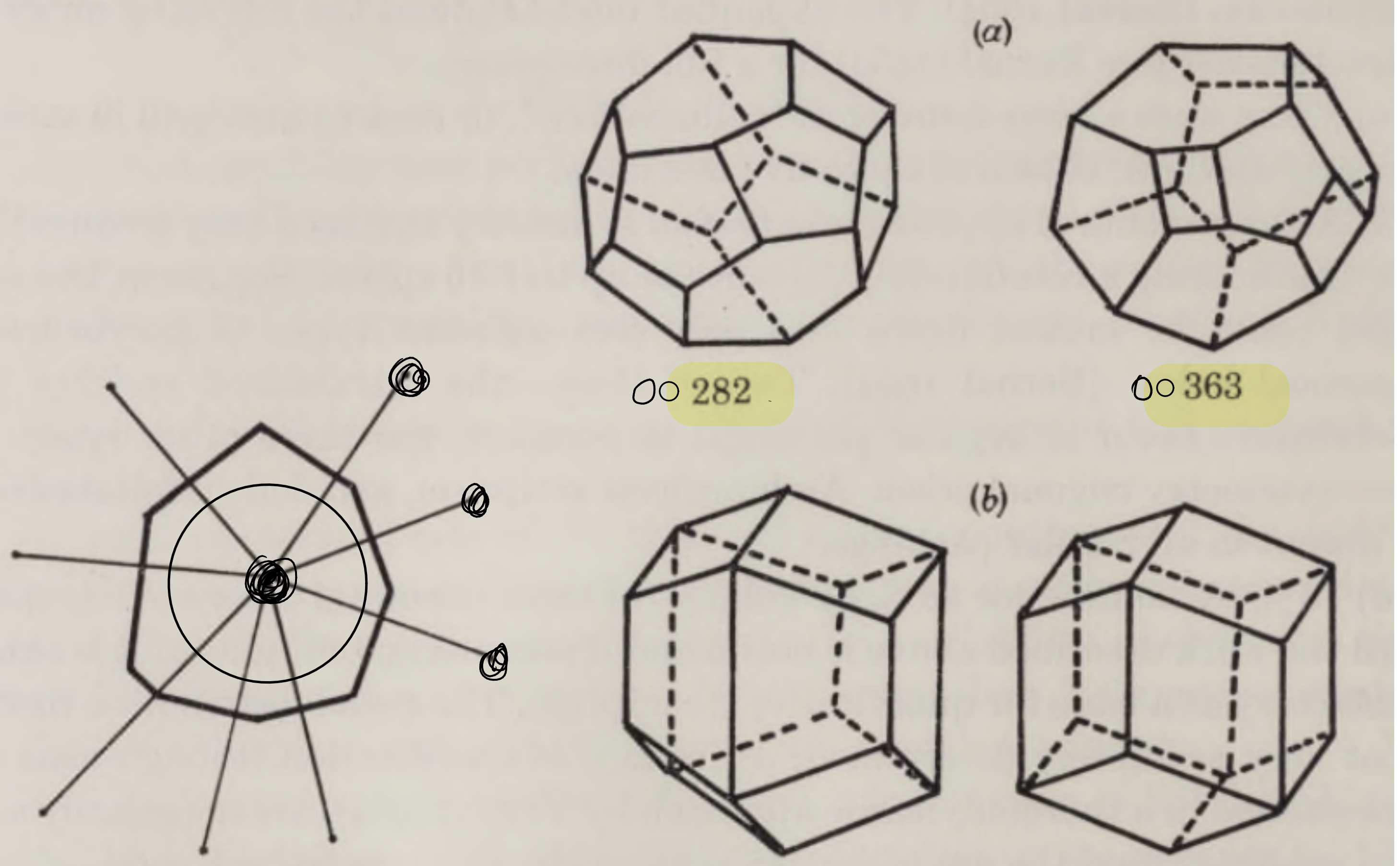


FIGURE 1 FIGURE 2

FIGURE 1. Construction of a two-dimensional Voronoi polygon.

FIGURE 2. (a) Two typical irregular Voronoi polyhedra. (b) Two regular Voronoi polyhedra, derived from hexagonal and cubic close-packing respectively.

Finney & Bernal 1972

Random close packing

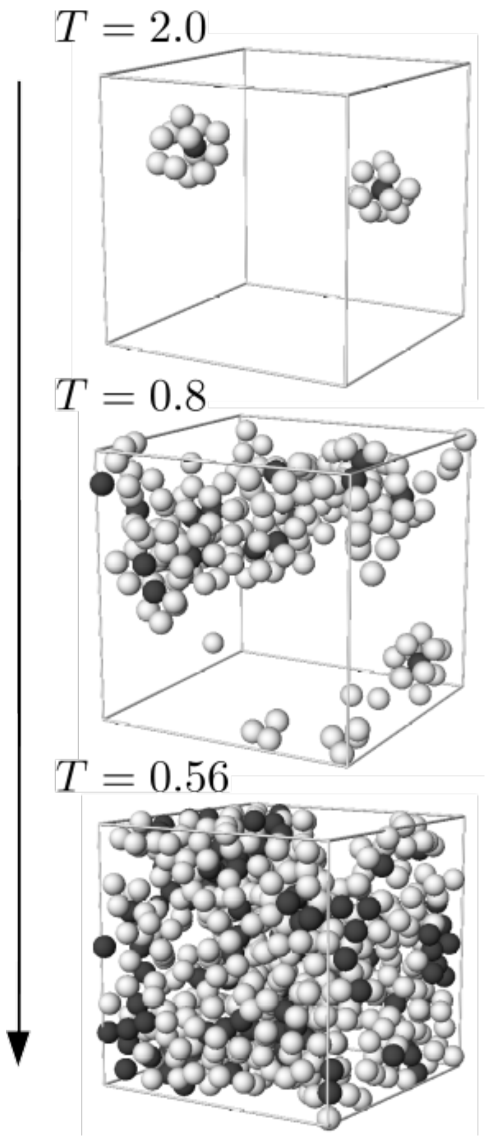
Congettura Eulero : $\phi_{FCC} = 0.74$

$\phi_{RCP} \approx 0.64 - 0.68$

Packing isostatici : $dN = \frac{1}{2} N z$

$z = 2d$ → JAMMING

Struttura localmente favorita (LFS)



Hansen, Barrat, Pastore

$$u_{\alpha\beta}(r) = \epsilon_{\alpha\beta}\left(\frac{\sigma_{\alpha\beta}}{r}\right)^{12}$$

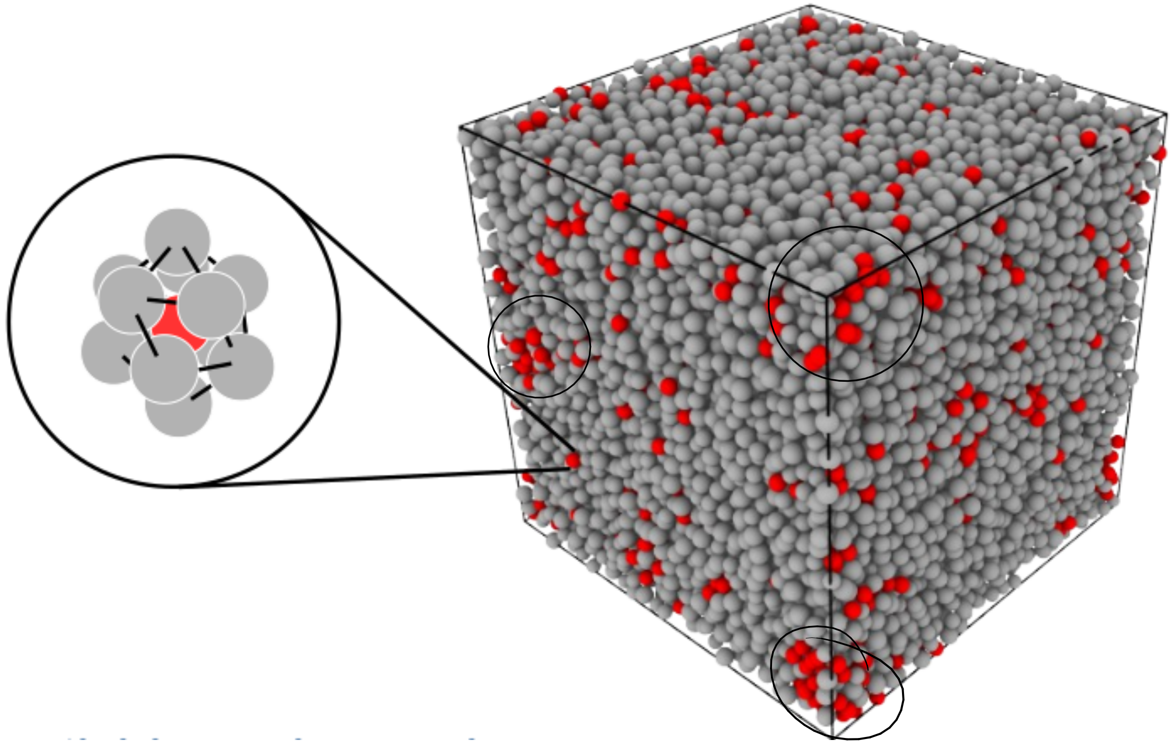
$\frac{\sigma_{AA}}{\sigma_{BB}} = 1.4$ $\quad \epsilon_{AA} = \epsilon_{BB} = \epsilon_{AB}$

$\frac{\sigma_{AA}}{\sigma_{BB}} = 1.2$ Wahnström

$T_{onset} \approx 1.0$

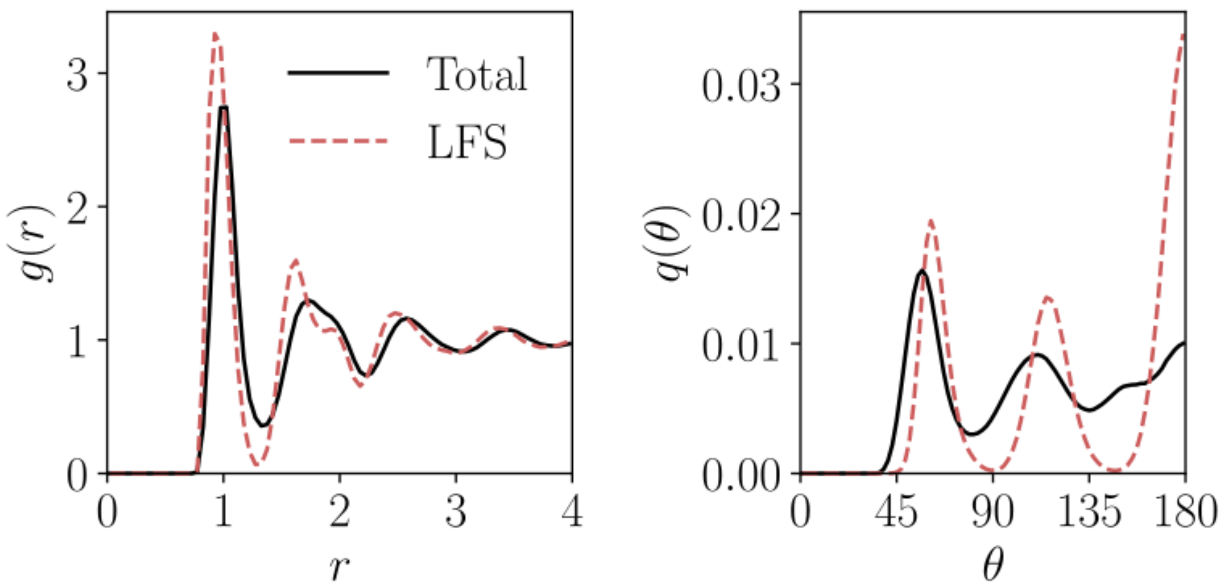
$T_c \approx 0.55$

⚠ $MgZn_2$

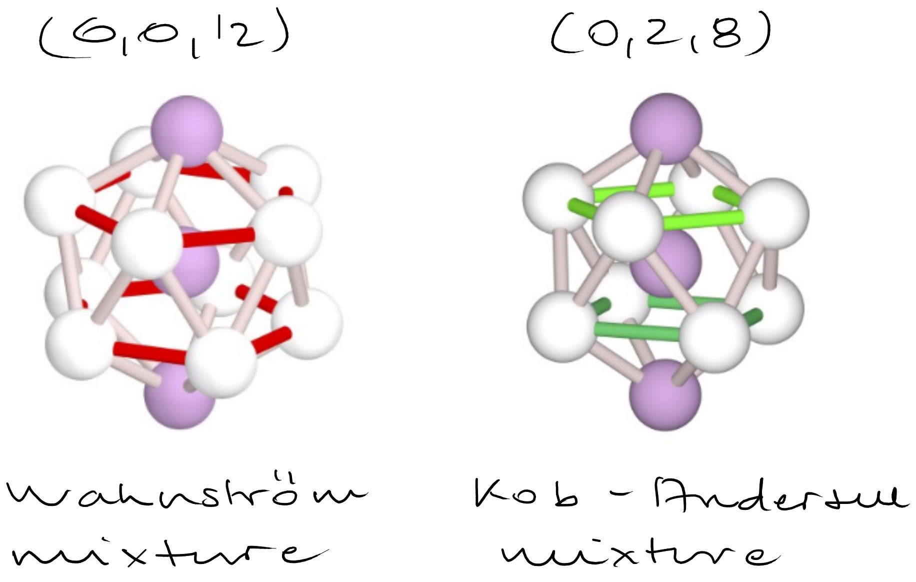


Wahnström

Coslovich Pastore JCP 2007

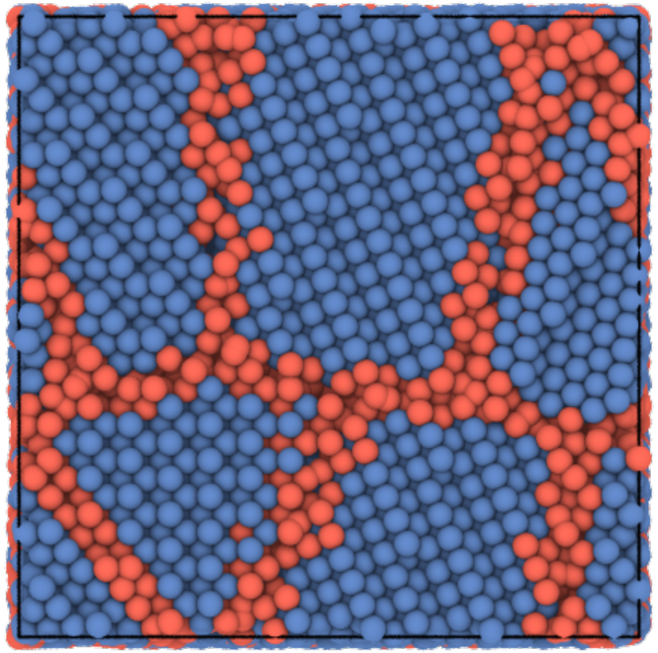


→ community inference JCP 2019




```python
from partycls import Trajectory, Workflow

traj = Trajectory('grains.xyz')
wf = Workflow(traj, descriptor='ba', clustering='kmeans')
wf.run()
traj[0].show(color='label', backend='ovito')
```



partycls

https://github.com/jorisparet/partycls