Debye used kinetic theory of Gas Analogy

$$K_i = C_v v_m \Lambda / 3$$

$$v_m = 3^{1/3} \left(\frac{1}{v_p^3} + \frac{2}{v_s^3} \right)^{-1/3} \approx A \left(\frac{E}{\rho} \right)^{1/2}$$

longitudinal & transverse wave velocities

let $\frac{M}{m} =$ $\frac{\text{Molecular mass}}{\text{\# atoms per molecule}}$

~~$A = 0.87 \pm 0.02$~~ but E within 20%

$$K_{min} = 0.87 k_B N_A^{2/3} \frac{m^{2/3} \rho^{1/6} E^{1/2}}{M^{2/3}}$$

→ minimize K, look @ parameters

- large molecular weight
- complex crystal structure
- ~~bonding~~ non-directional bonding
- large # of different atoms per molecule
- low modulus

→ exception: SiO_2

- dopants further scatter phonons inelastically
  by analogy same as Rayleigh light scattering
  from defects, pores, ~~etc~~. vacancies etc..
  - (isotopically pure carbon = high K)
- alloying, mass disorder $NiO - MgO$
  $In - GaAs$
  $Ge - Si$
- flexible structures (SiO_2)
  corner shared polyhedra
  phonon mean free path limited to SiO_4 tetrahe
  - disorder at variety of length scales

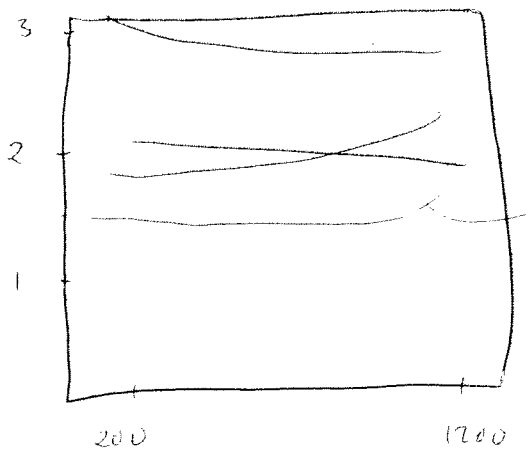
Reducing K in YSZ

8 m/o $YO_{1.5}$ has vacancy spacing ~1.25 nm
at higher concentration clustering of vacancies occurs

→ Zhu & Miller added other trivalent 3^+ cations
like Tm^{3+}, Eu^{3+} which have ~~XXXX~~ $M \tilde{=} 170, 150$ g/m
compared to 89 g/m (Y^{3+} "Cluster Doped"

→ Clarke: try to disorder Zr^{4+} lattice! Hf^{4+} is
same size, twice as heavy.

~~a) dissolution pressure SnO_2 < 800~~



7 YSZ

7 YSZ + 3.5 $EuO_{1.5}$ + 3.5 $YbO_{1.5}$

" " + 3.5 " + 3.5 $TmO_{1.5}$

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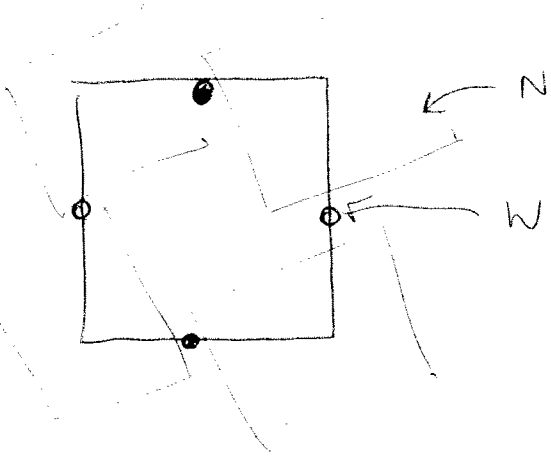
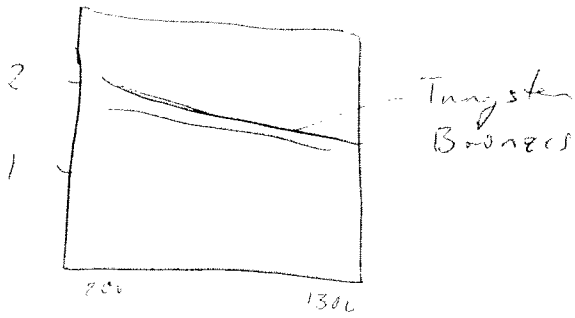
try "SiO_2-like" structure

Nb-W-O Tungsten bronzes





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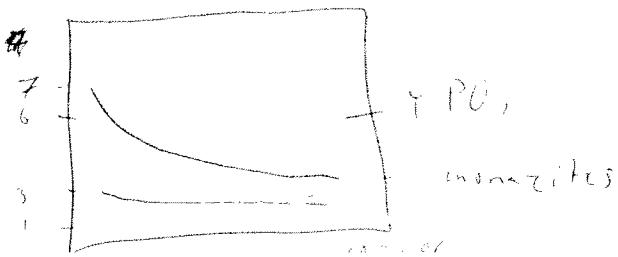
try $LnPO_4$ which is isostructural to SiO_2

but PO_4 instead of SiO_4

$(La_{0.5}\ Gd_{0.5})PO_4$ vs YPO_4 both have equal interatomic distance

it depends on how polyhedra connect!



Xenotime (YPO_4) | monazite ($GdPO_4$ or $LaPO_4$)

REO_8 – high symmetry
- equal bond lengths
- no rotational polyhedra (all parallel)
- some edge sharing
=> more ordered

REO_9 ← weaker bonds
← bond lengths vary
- rotated polyhedra along [00
- corner sharing only
=> less ordered

$La_2Mo_2O_9$ → high ionic conductivity → low K

LaO_9 } partially filled
MoO_7 } oxygen sites

→ large mean atomic mass
→ many vacancies and all are very mobile

$0.75 \frac{W}{mK}$

no T dependence

compound	Σ_2
7.45 Z	0.1158
YPO_4	0.1194
$LaPO_4$	0.1278
$Zr_3Y_4O_{12}$	0.1368
$Gd_2Zr_2O_7$	0.1350
$W_3Nb_{14}O_{44}$	0.1385
$La_2Mo_2O_9$	0.1410