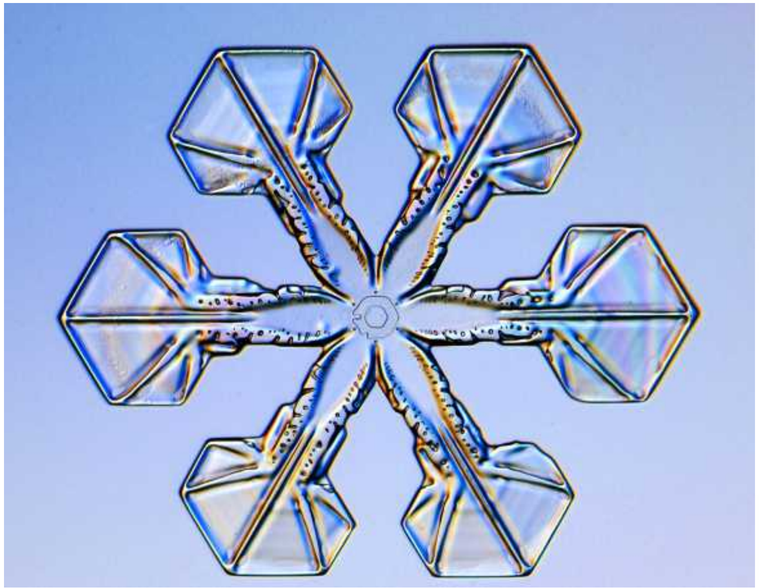
Particles, characteristic, sort

Contents of lecture

- 1. Characterics of particles
- 2. Percolation
- 3. Number of particles in composite
- 4. Influence of particles on matrix
- 5. Curiosity of nanoparticles

Forms of snowflakes



d_s = 0,5 mm

$D = 1/d_s = 2*10^5\ m^{-1}$

Snowflake have cca 1/10 volume of sphere

Surface of snowflake is more then ten surfaces of sphere

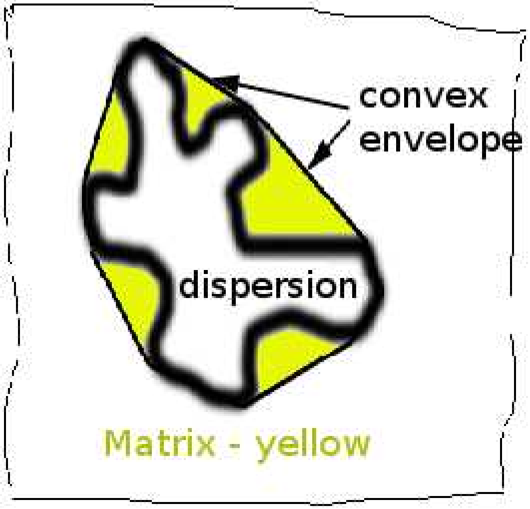
Ratio of surface to volume of snowflake $S = 10^8\ m^{-1}$ (m^2/m)

Characteristic of particle - convexity

Determines possibility of mechanical coupling of particle in matrix.

Coefficients of convexity :

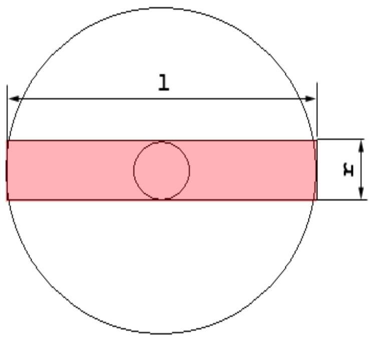
- C_1 = (surface of particle) / (surface of convex envelope)
  - exact
- C_2 = (surface of cross section of particle) / (surface of convex envelope)
  - from cut
  - practical, not exact



Characteristic of particle – isometry

Characteristic of ability to have no significant direction (without significant orientation) – result is isotropy of composite

Coefficients of isometry :



- $F_1 = 4*\pi*$ (area of cross section) / (circumference of cross section)^2
  ball $F_1 = 4*\pi*(\pi r^2)/(2\pi r)^2 = 1$
  cube $F_1 = 4*\pi*(a^2)/(4a)^2 = \pi/4 = 0{,}79$
  long bar $F_{1k} = 4*\pi*(\pi r^2)/(2\pi r)^2 = 1$ … transversal
  $F_{1o} = 4*\pi*(rl)/(2*(l+r)^2 \approx 2*\pi*r/l \rightarrow 0$ … axial
- F_2 = radius of inner circle / radius of outer circle
  ball F2 = 1
  cube F2 = $1/\sqrt{2} = 0{,}71$
  long bar $F_{1k} = r / r = 1$ $F_{1o} = r / l \rightarrow 0$

Characteristic of particle - size

- Sieve analysis - **dimension d_s** – diameter of sieve opening, into which particle sink – only upper limit (maximum)
- Specific surface - S = surface / mass of particle from assumption ball or cube

$$S = 6a^2 / \rho a^3 = 6/(\rho * a)$$

Equivalent diameter **$d_p = 6 /(\rho * S)$,**

ρ … density, better simple $d_p = 6 * V/F$,

V … volume and F … surface of particle

- Degree of dispersity **D = 1 / d (m^{-1})**
  - from physical chemie

  Particle of ball or cube shape 1 µm great has dispersity $D = 10^6\ m^{-1}$

Characteristic of particle - distinguishable

With optical microscope
- d > 1 μm, D < 10^6 m^{-1}, particle

Scanning electron microscop
- SEM - 0,1 bis 1 μm, microparticle, D = 10^6 až 10^7 m^{-1}

TEM - below 100 nm,
nanoparticle, D > 10^7 m^{-1}

Distance of particles

regular square arrangement

Free distance between particles

$S_{min} = a – d$, $S_{max} = a*\sqrt{2} – d$

Volume particle concentracion

$v_d = (\pi d^2/4) / a^2$

By integration from S_{min} till S_{max} ve can calculate mean free distance between particles

$S = \sqrt{(2/3)}*d /\sqrt{v_d}$

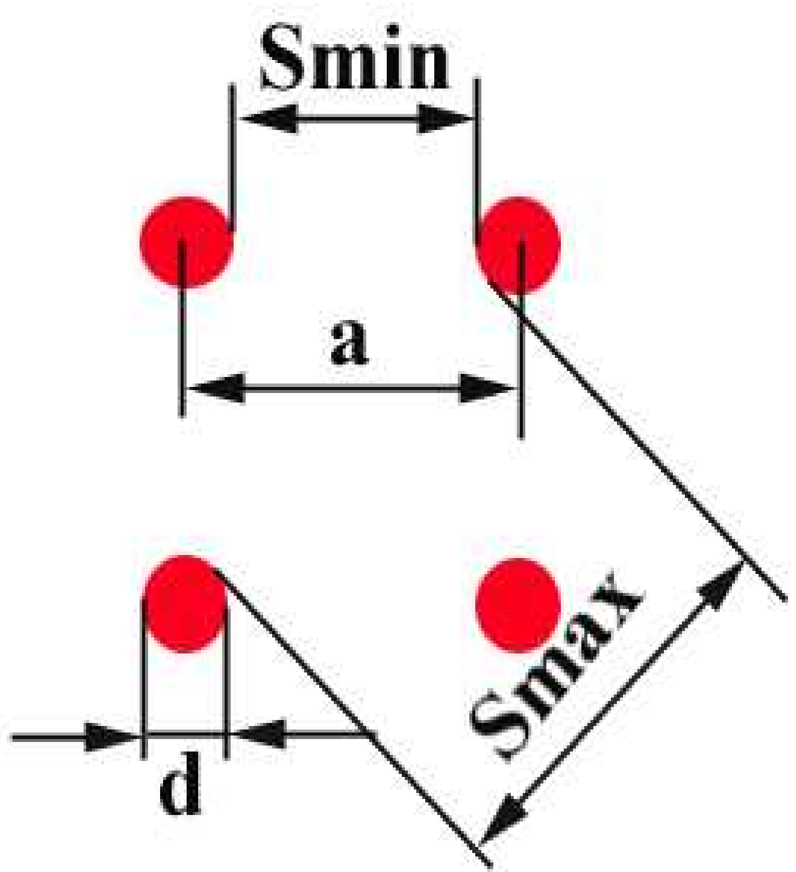
Because

$S_{min} = d*((\sqrt{\pi} /(2\sqrt{v_d})) -1)$,

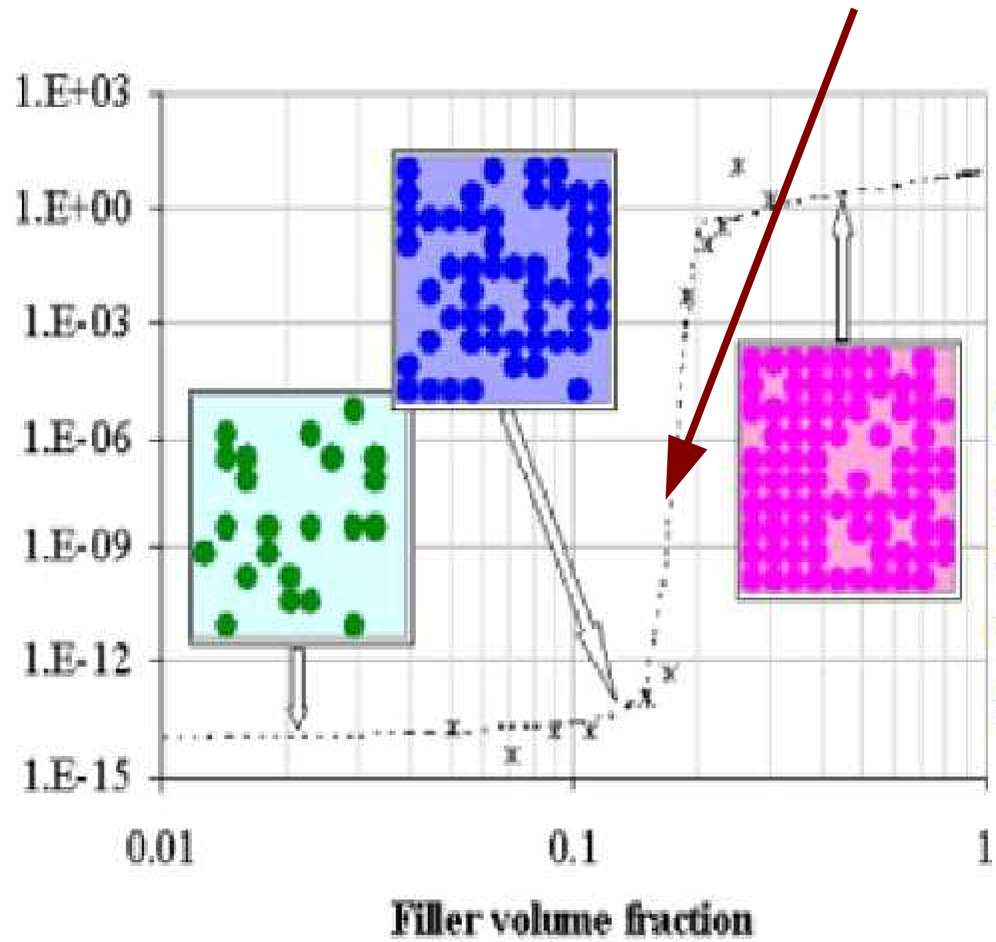
for $S_{min} = 0$ we have

$v_d = \pi/4 = 0,785$,

above that concentracion are all particles in contact.



Percolation limit



$$\sigma_c = \sigma_f \left(\phi_f - \phi_c\right)^s$$

σ_c – conductivity of composite

σ_f – conductivity of dispersion

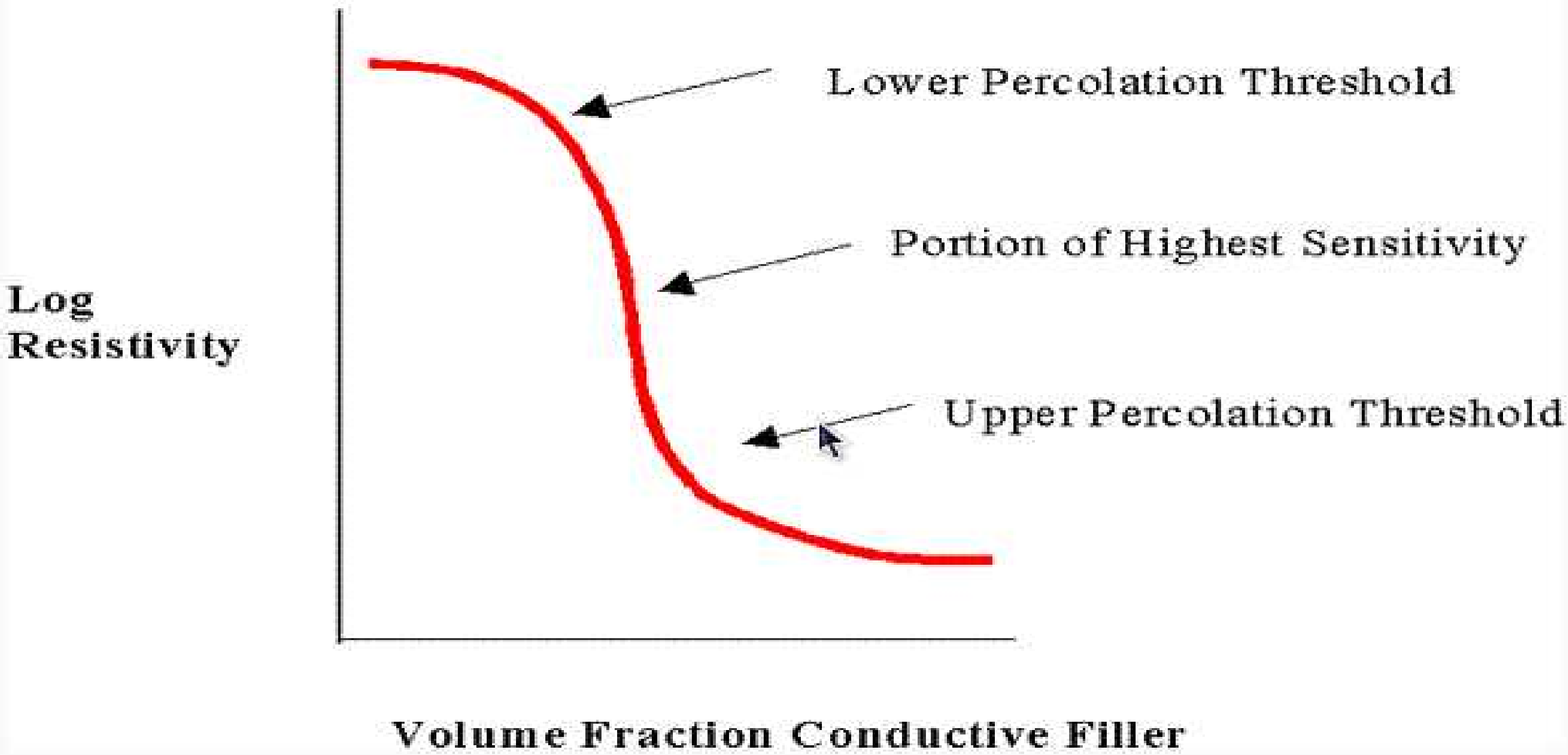
Φ_f – concentracion of dispersion

Φc – percolation coefficient

s – percolation exponent

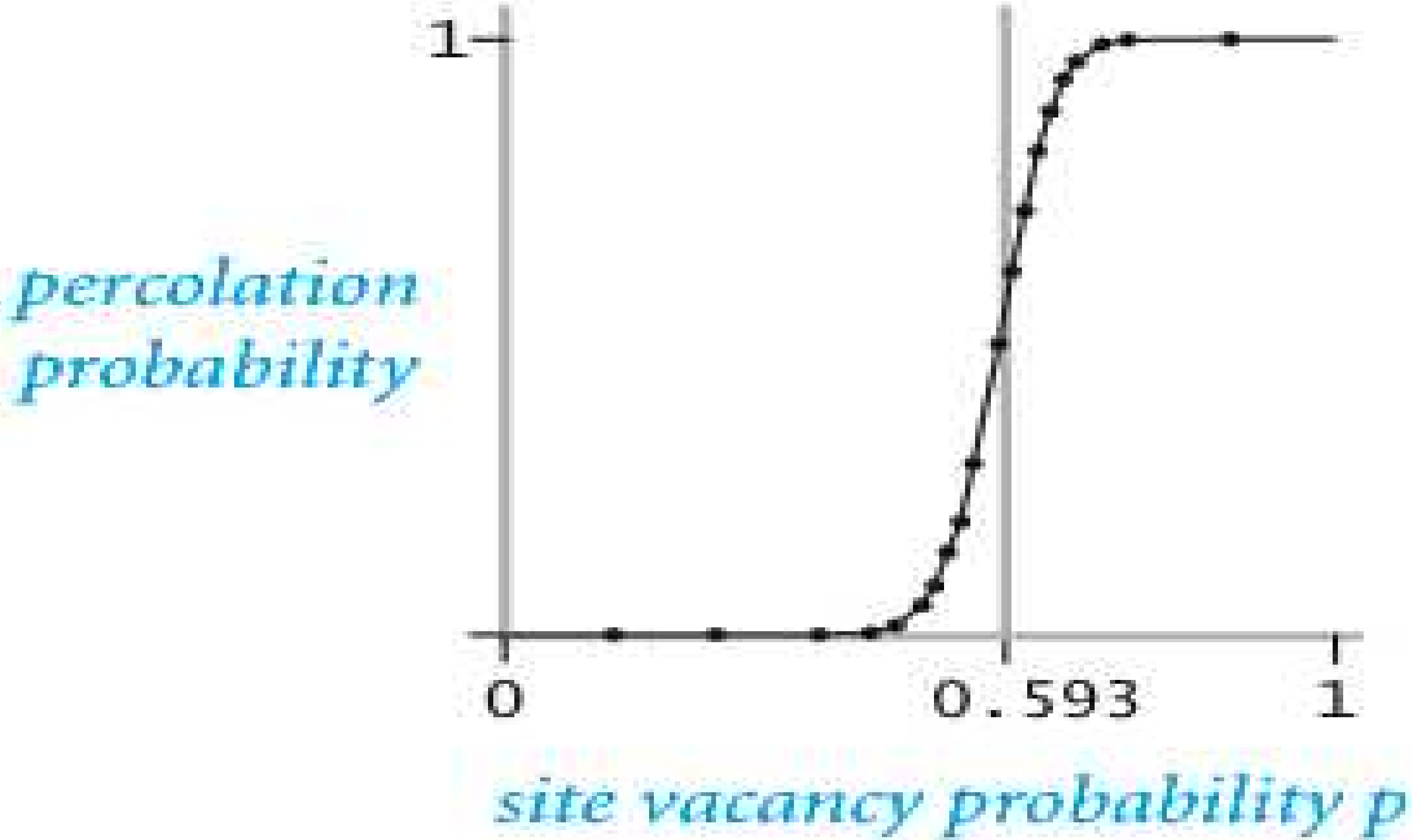
Results of electric conductivity simulation
– non-conductive matrix, conductive dispersion

Example of percolation curve



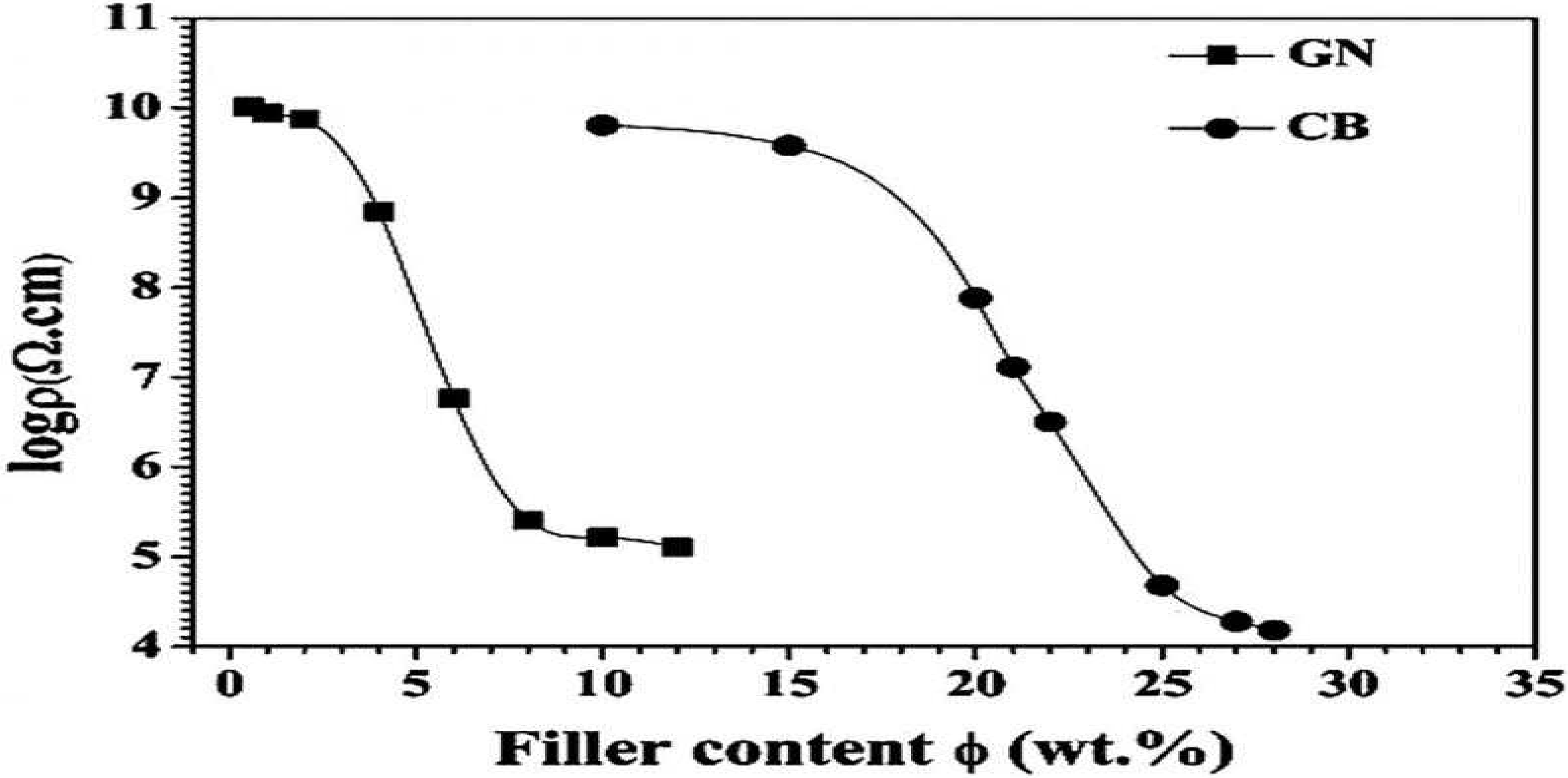
Valid for electric and thermal conductivity, hardness, by pore for gas permeability

Results of simulation



Princeton – square pore, permeability of plate

Effect of particle size



Electric resistance, matrix HDPE,
CB ... soot, GN ... graphene nanoflakes
(Guohoa Chen, 2010)

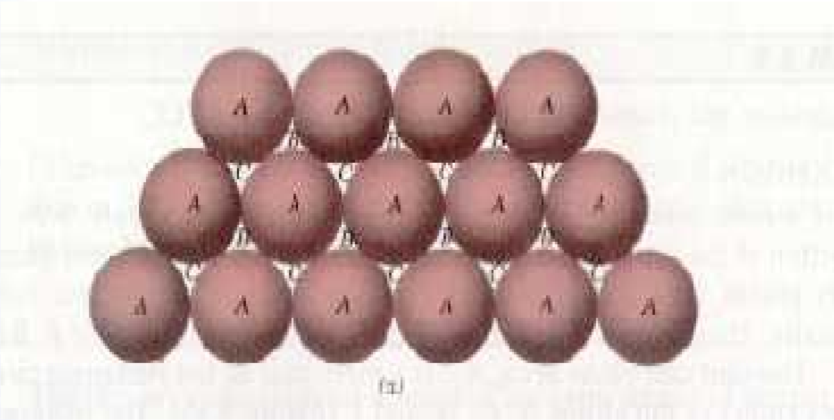
Closely packed particles

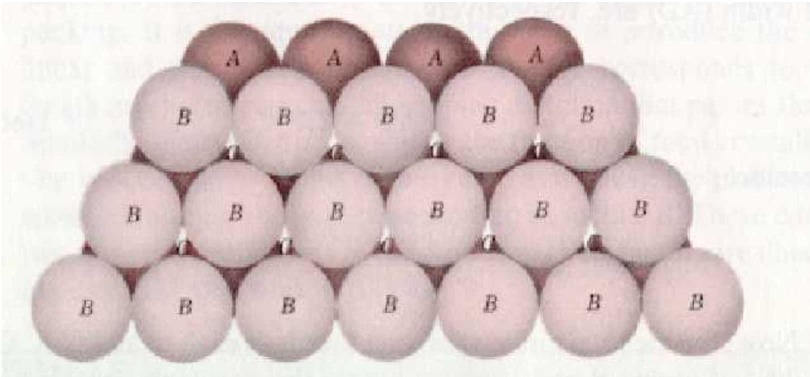
Quantity of particles – always volume %.

Assumption of globular (isometric) particles.

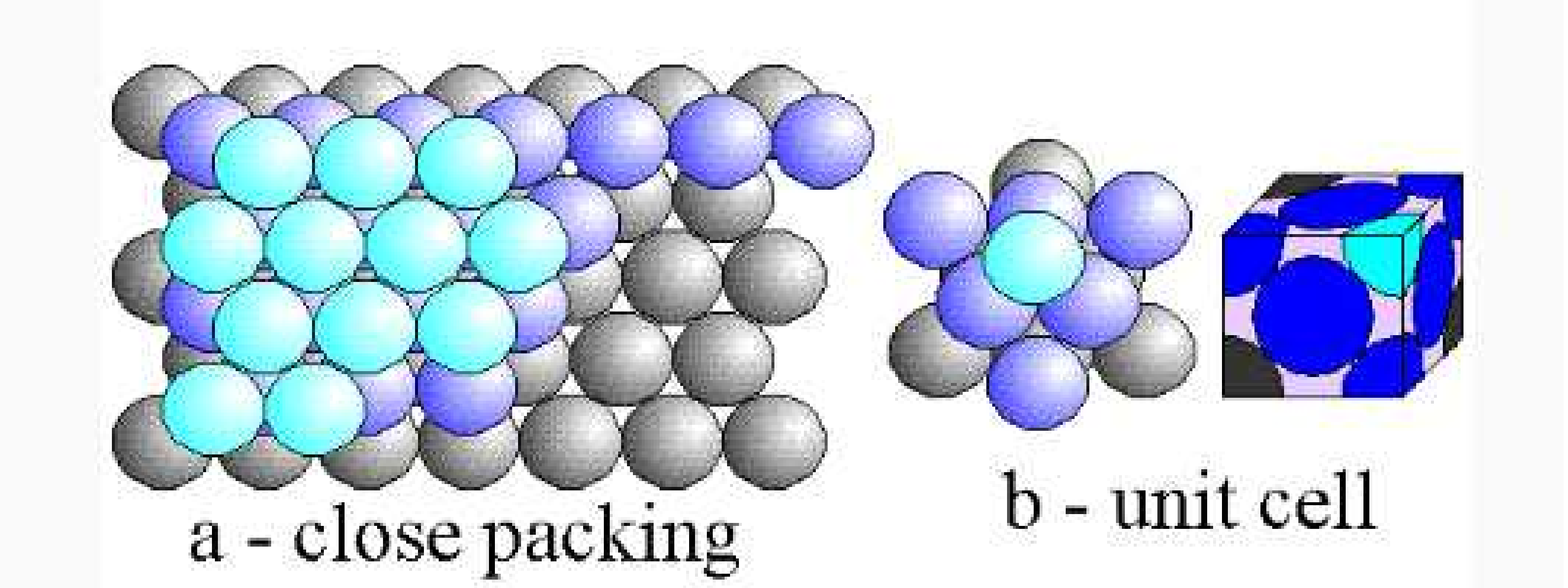
Closely packed on plain - equilaterale triangles

In space – the same plains sitting one on other – from the side the same picture





Another picture on close packing



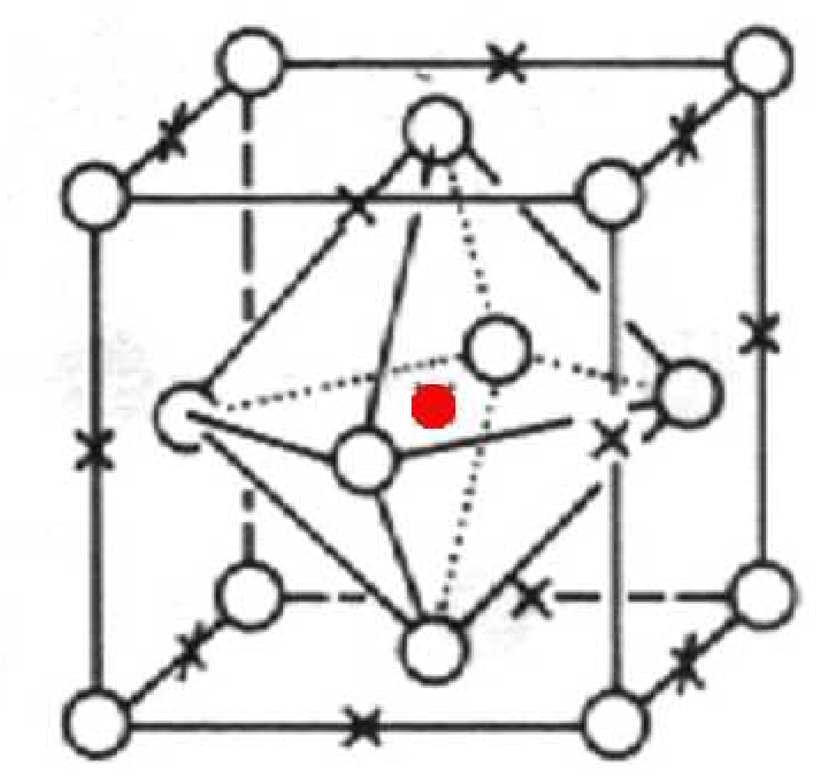
Radius of particle … r
Diagonale of side of cube 4*r, its edge 4*r/√2
Volume of cube $64*r^3/(2*\sqrt{2})$
Inside four ball particles $4 * 4/3*\pi*r^3$

Maximale concentracion of particles

- Particles could be maximal in clouse packing
  - that is 74 % of particle dispersion a 26 % of matrix
- If is more of particles, could be leeks in matrix, that leeks are closed
- There is theoretical calculation :
  - particles are never quite perfectly arranged
  - particles have not perfect ball shape
- In practice are in composites leeks already above 55 – 60 % particles
- Quantity of matrix in composite must be above 35 až 40 volume percent, to have composite without leeks

Maximale size of leeks

Red – octaedric void in cube – maximal possible closed leek.
Its radius 0,41*r
Also in cube vith volume $64*r^3/(2*\sqrt{2})$ is volume of particles
$4 * 4/3*\pi*r^3$
and volume of leeks
$0,41 * 4/3*\pi*r^3$



Connecting of leeks

By maximal shape of leeks from previous picture composite have in 100 % volume 74 % particles, 18,5 % leeks and only 7,5 % matrix.

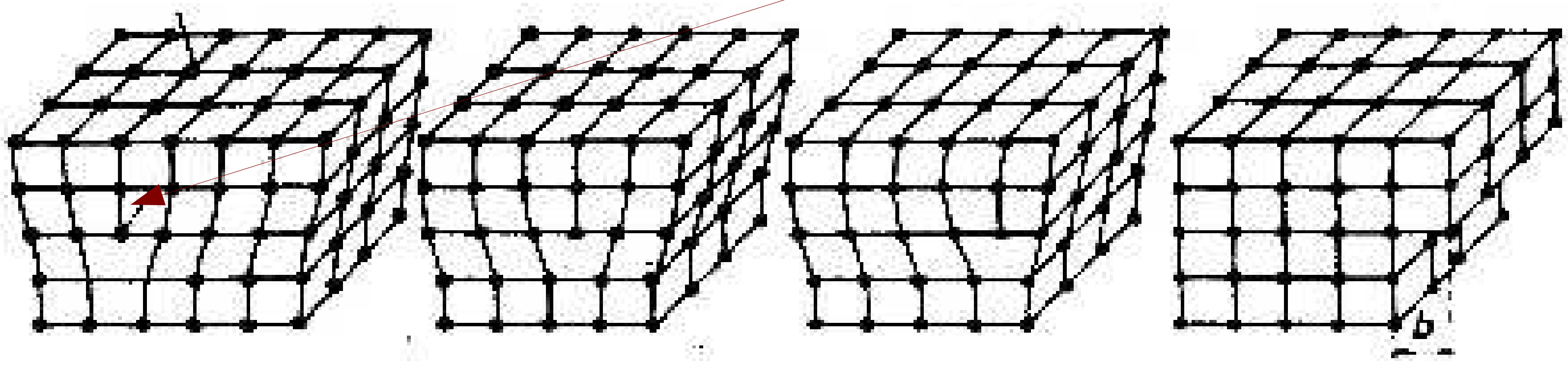
If is concentracion of matrix above that quantity, leeks are closed in inner of composite.

If is concentracion of matrix below that quantity, leeks begin to connect and create in composite microchannels – capilarries. Composite is becomming permeable for fluid and gas.

Again theoretical calculation - in practice are in composites leeks in microchannels already above 70 % particles.

Plastic deformation of composite

- Particles can hinder plastic deformation.
- Main cause of plastic deformation is movement of line defects - dislocations



Movement of dislocation

Strenghthening due to armour

Great particles could not hinder movement of dislocation (dislocations can walk around particles), but take part of forces.

Optimum – particles above 1 μm, aproximately 25 %. By greater quantity of patricles – tearing of matrix.

Near particles is hydrostatic pressure.

Brittle particles are due to that pressure deformable, crack above 3 * yield strength

By ductile particles due to that pressure decrease yield strength – they are sooner deformable.

Nanoparticles are very small for that effect.

Strenghthening due to dispersion

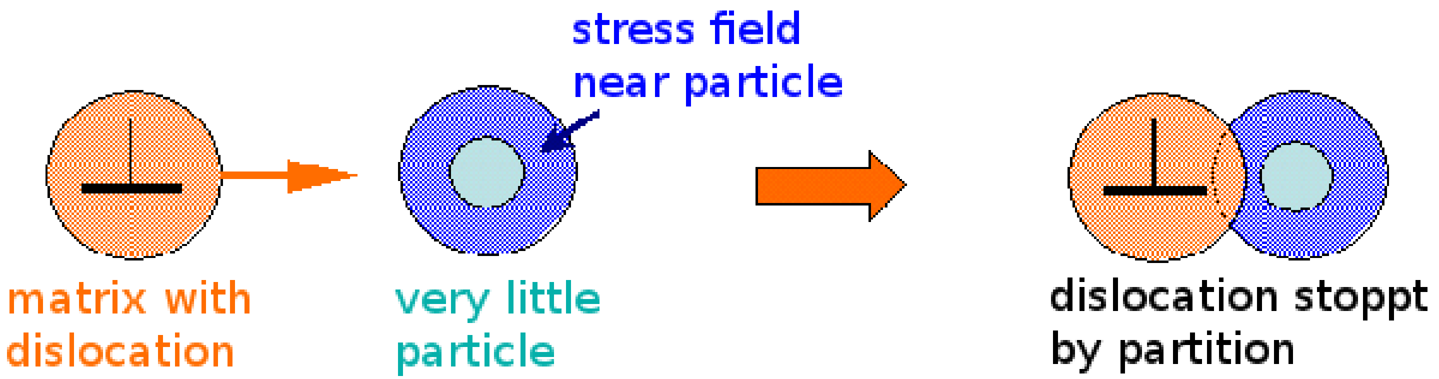
Stress necessary to movement of dislocations between micro – or nanoparticles is inverse proportional distance between particles.

Optimale distance and quantity of particles is composite with etwa 15 % nanoparticles with diameter near 100 nm.

Ultimate strength is not too increased, bud composite is very resistant to creep, bis 80 % melting point.

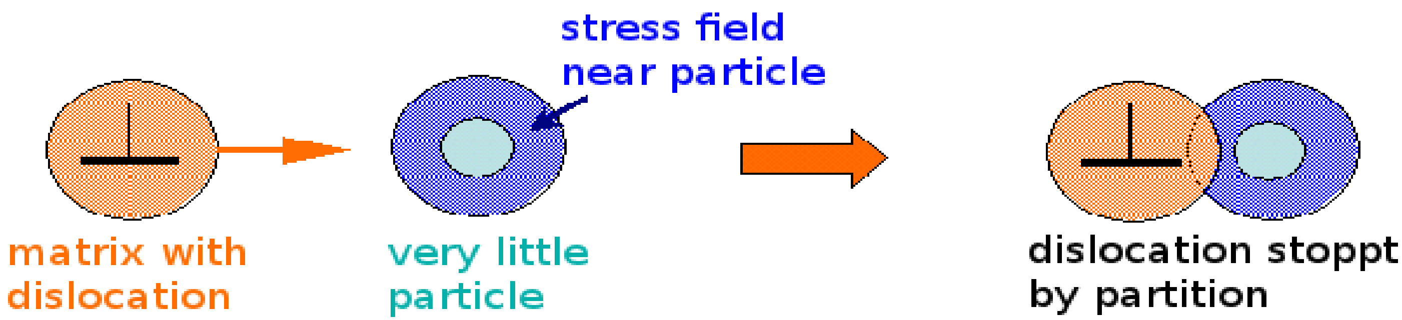
(usual metals bis 50 % melting point)

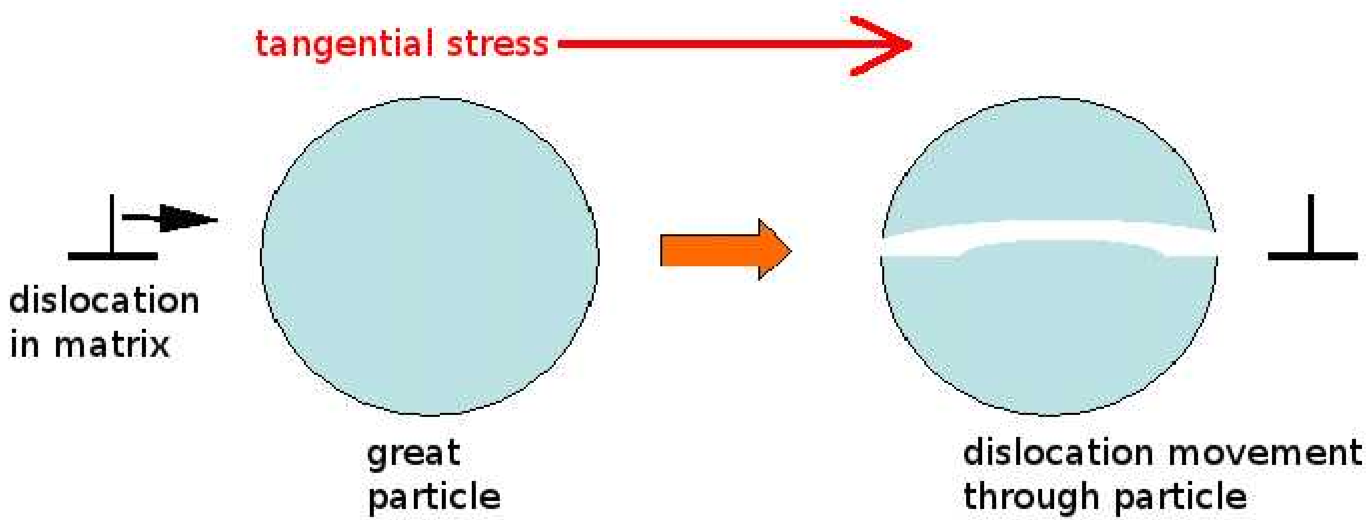
Examples : Cu - SiO_2, Fe - Al_2O_3, Ni - TiC



Comparison of strenghthening

Dispersion strenghthening





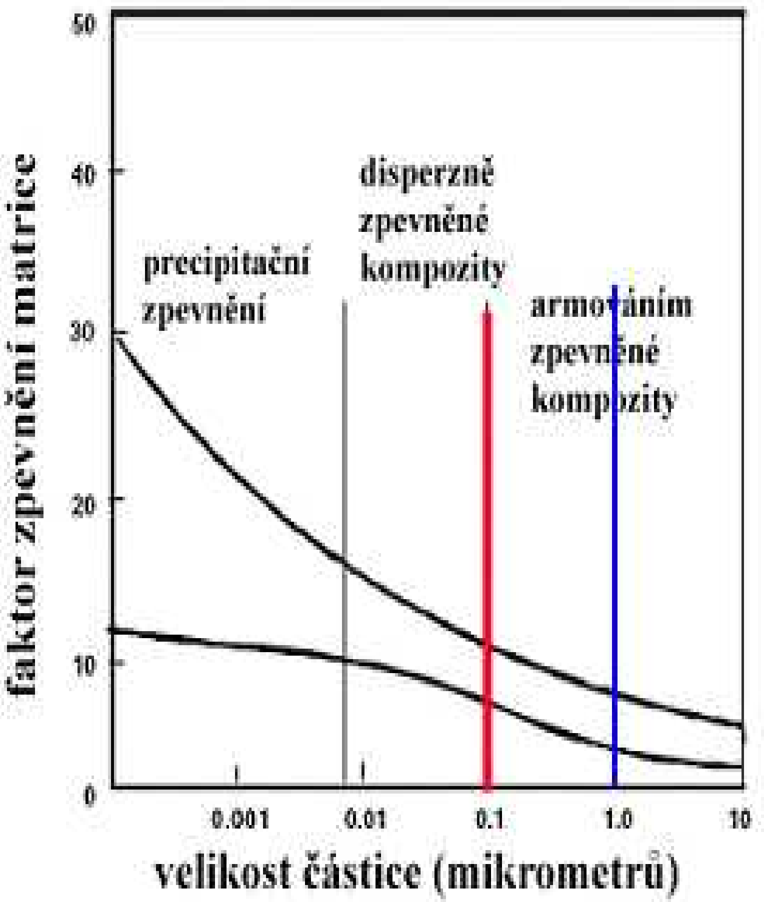
Armour strenghthening

Comparison of metal hardening

Precipitation hardening – typical by metals

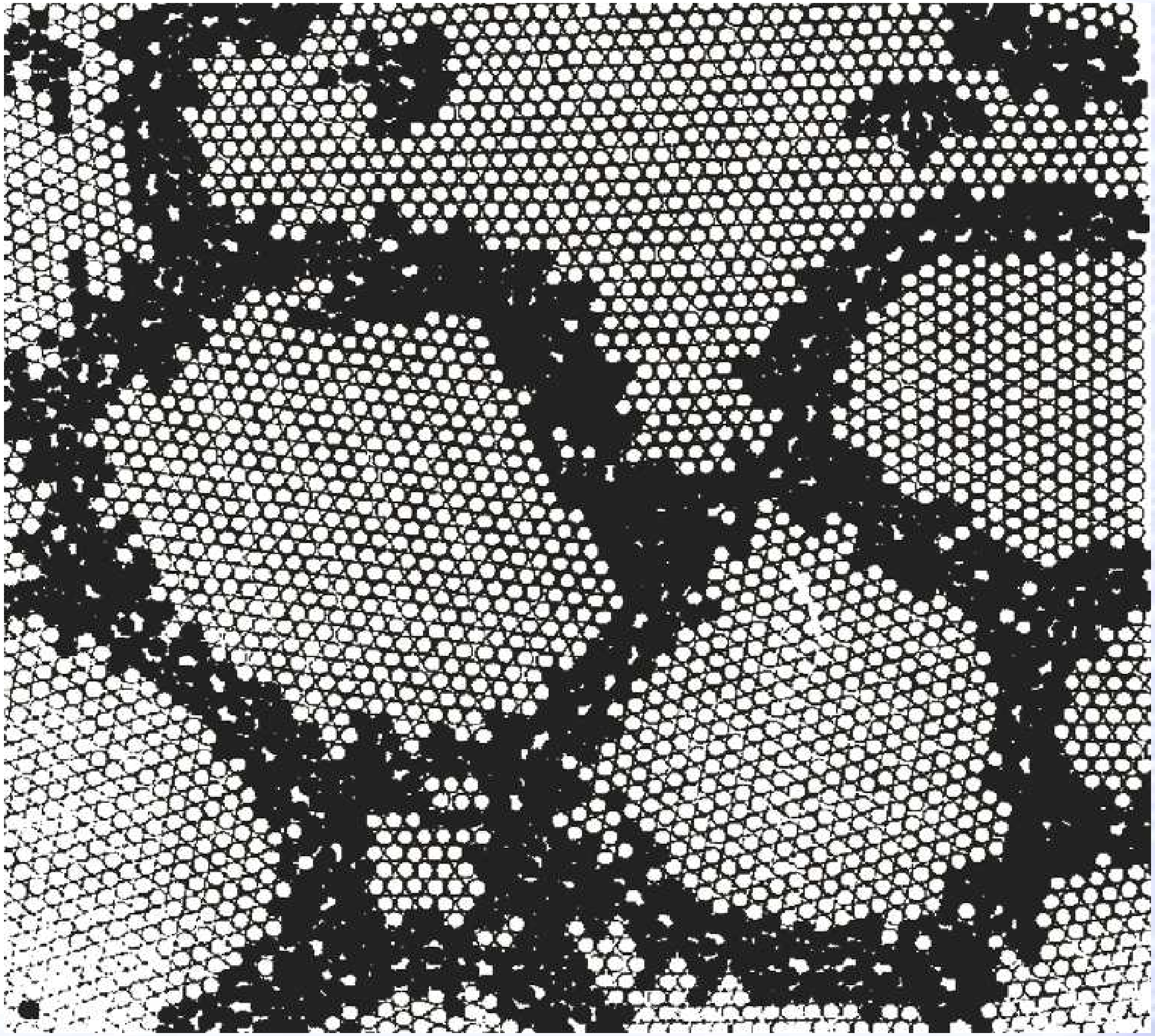
Dispersion hardening by composites
– red optimum

Armour hardening by composites
- blue optimum

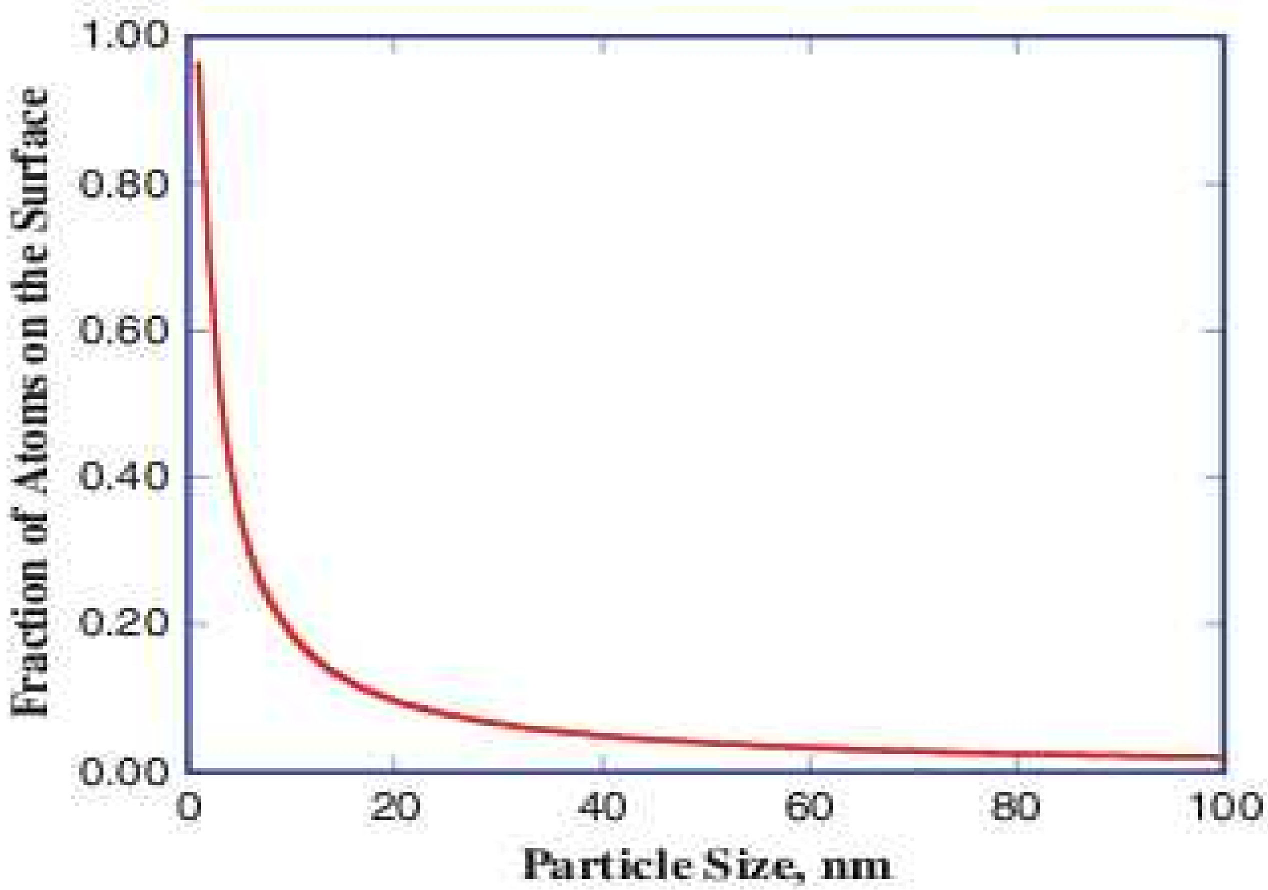


Nanoparticles

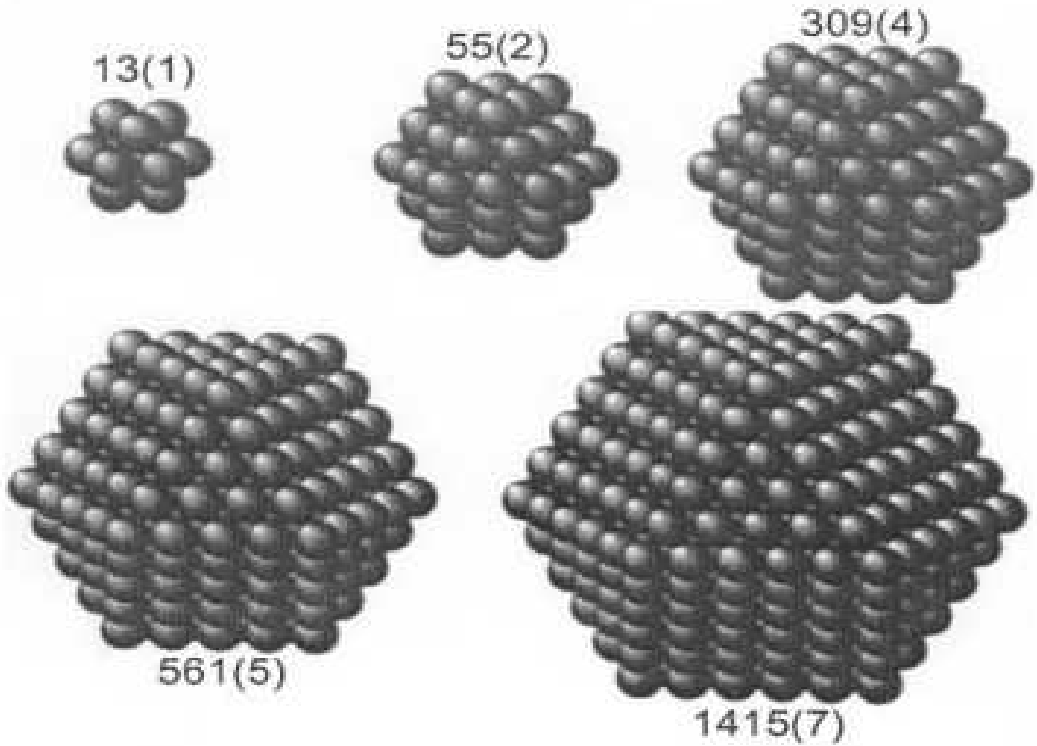
- Boundary layers :
  - more reactive
  - lower density
  - dispersion of interatomic distances



Fraction of surface atoms

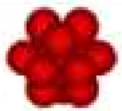
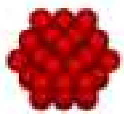
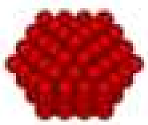
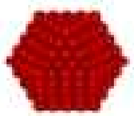
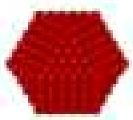
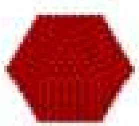


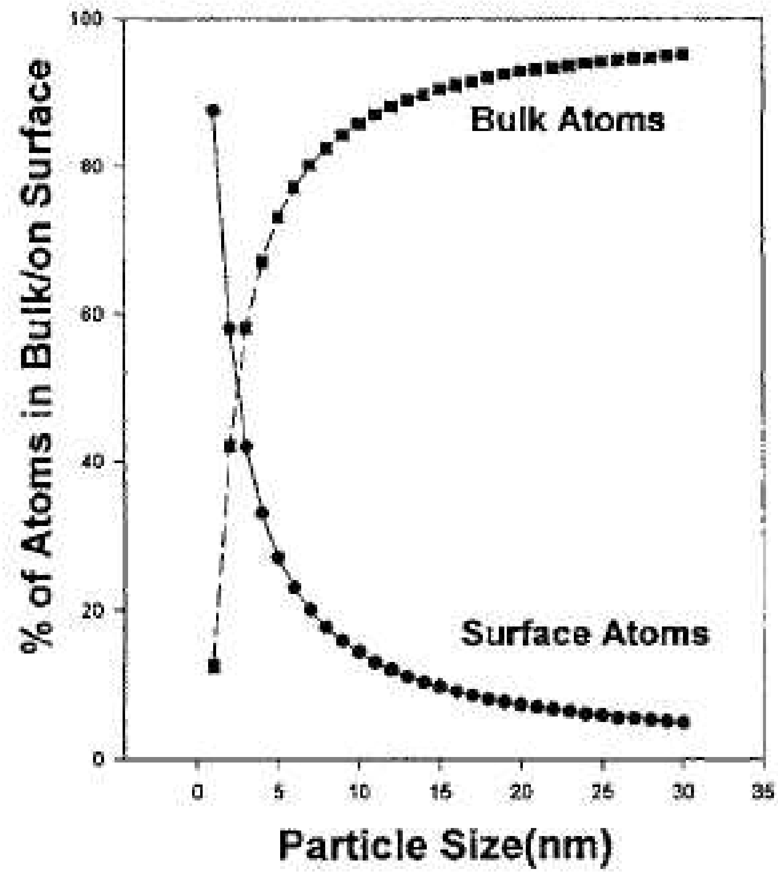
Nanocrystals – metal clusters



Metal nanocrystals in closed-shell configurations with a magic number of atoms. The number of shells is indicated in brackets.

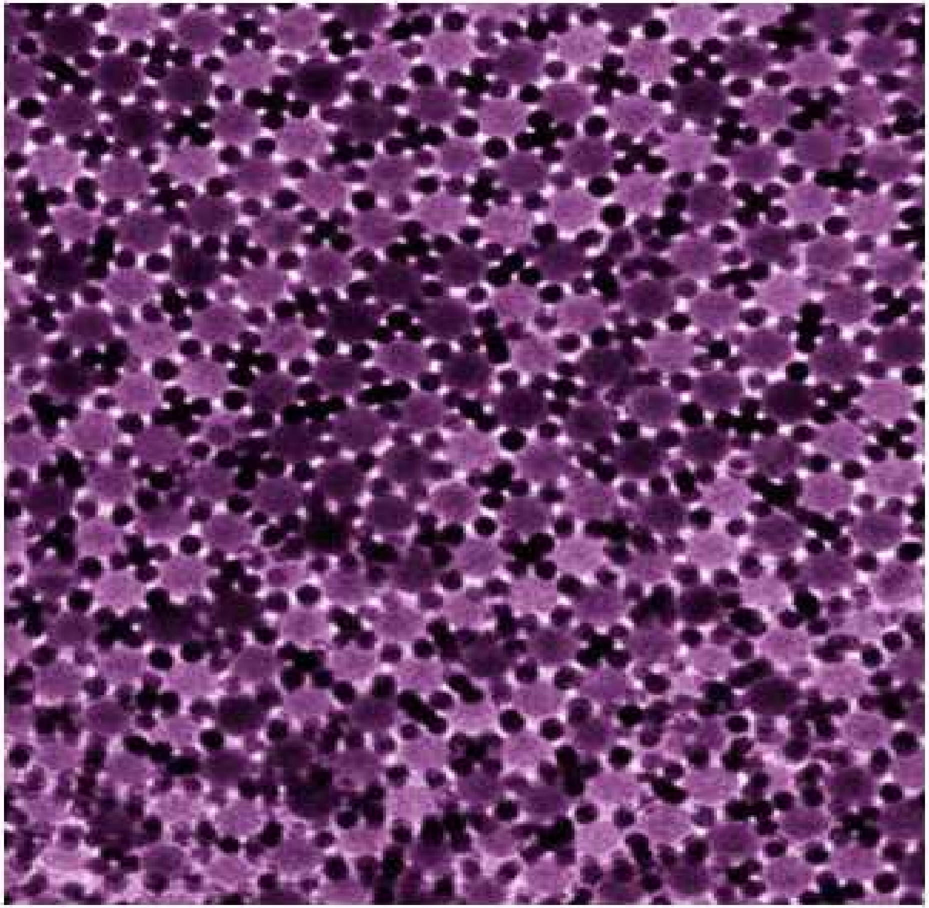
Surface of metal clusters

Full-shell Clusters		Total Number of Atoms	Surface Atoms (%)
1 Shell		13	92
2 Shells		55	76
3 Shells		147	63
4 Shells		309	52
5 Shells		561	45
7 Shells		1415	35



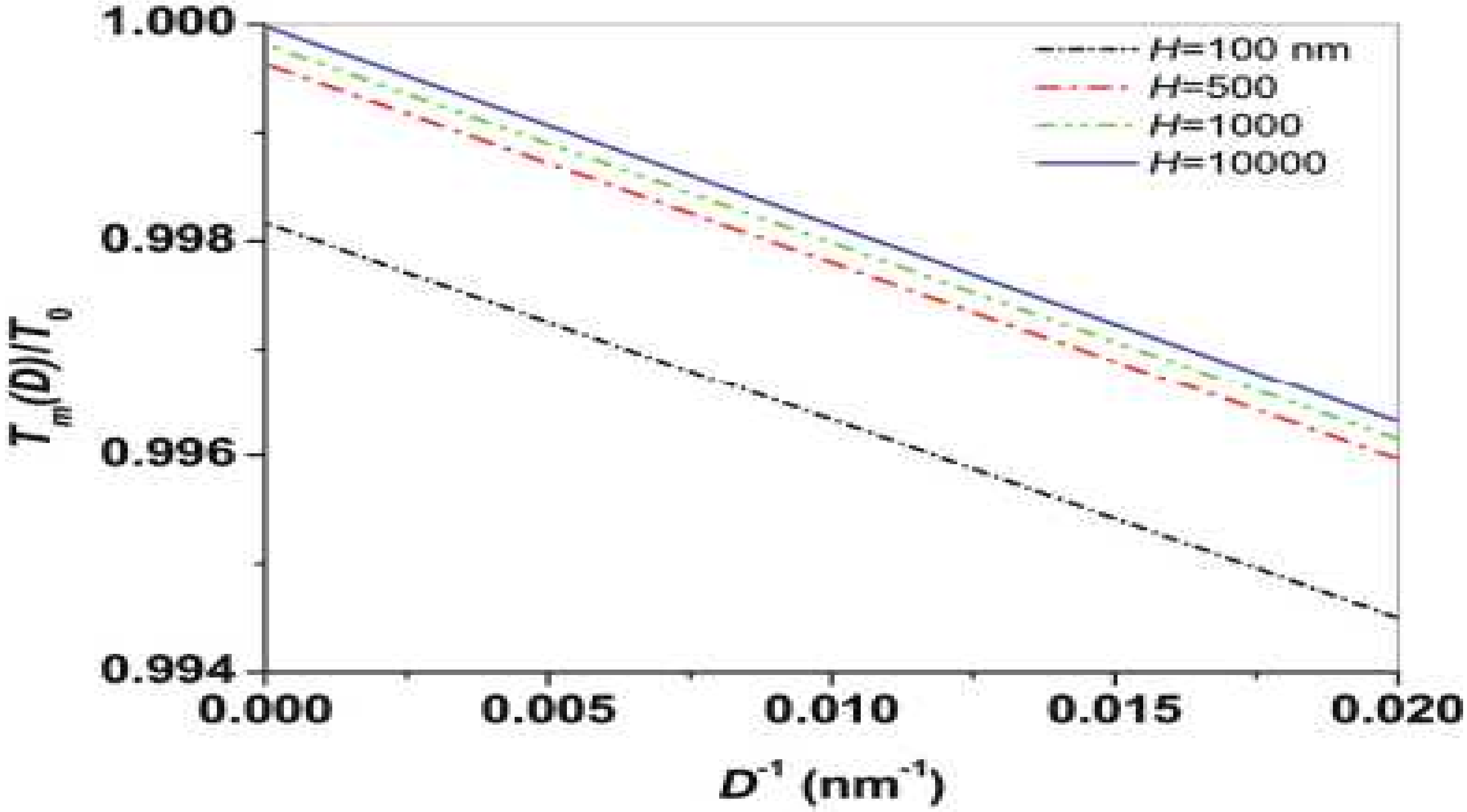
K.J. Klabunde (editor), Nanoscale Materials in Chemistry. John Wiley &Sons, Inc., 2001

Quasicrystals from nanoparticles - coagulation



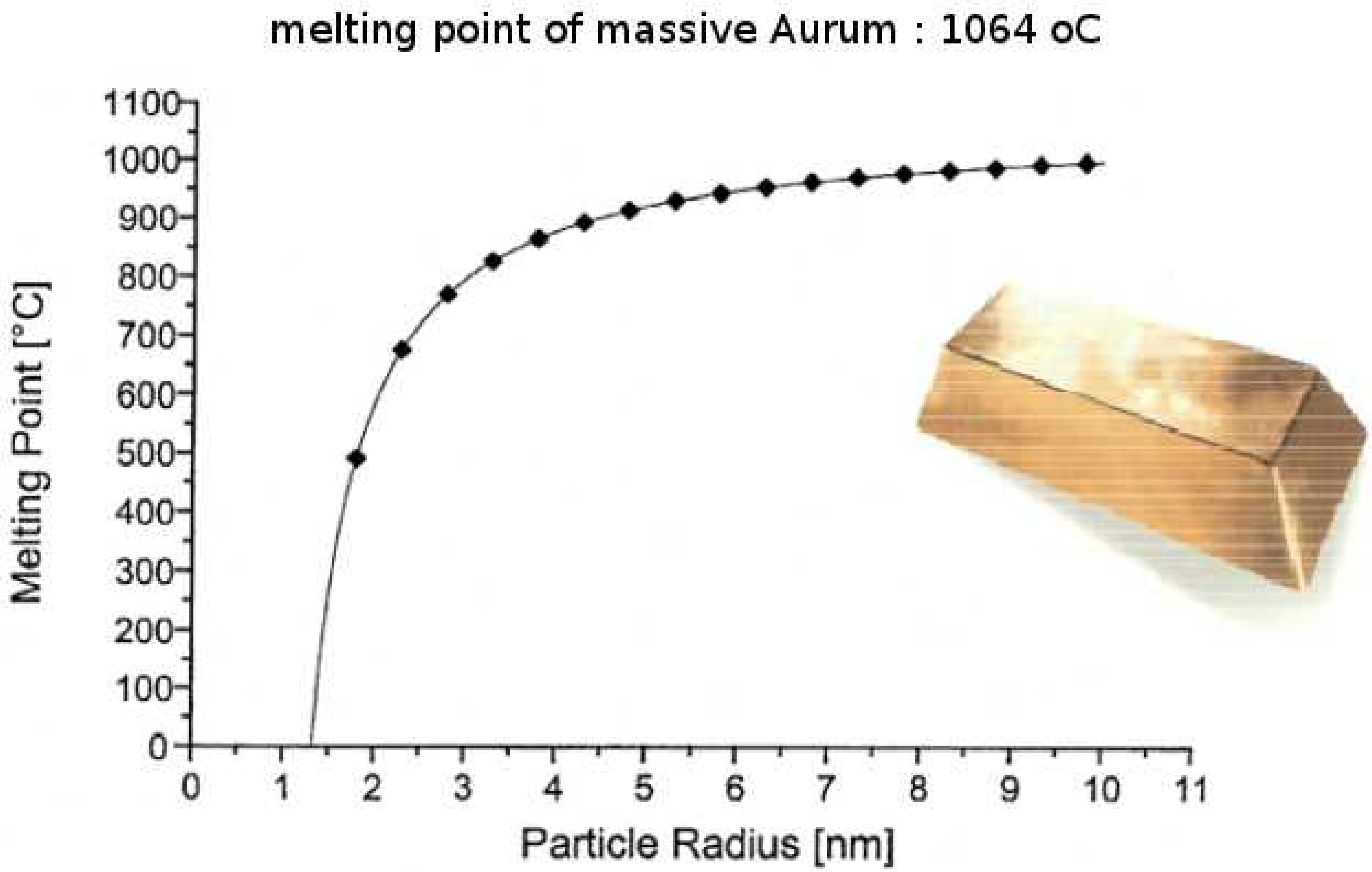
TEM showing the two-dimensional dodecagonal quasi-crystalline structure self-assembled from 5-nm Au and 13.4-nm Fe_3O_4 nanoparticles.

Dependence of melting point on particle size

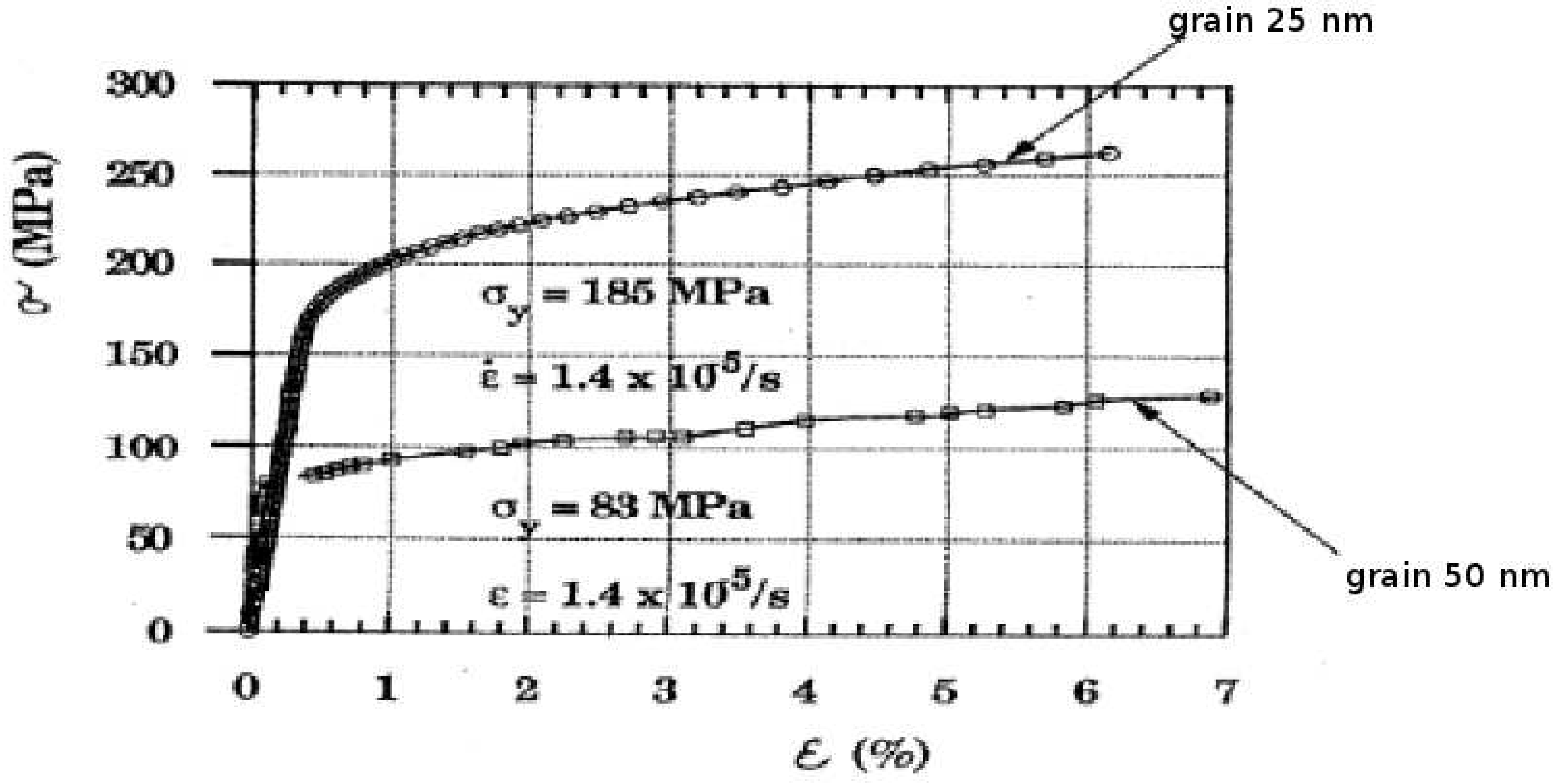


D ... edge of base, H ... high of prism. Termodynamic model.

Experimental dependence

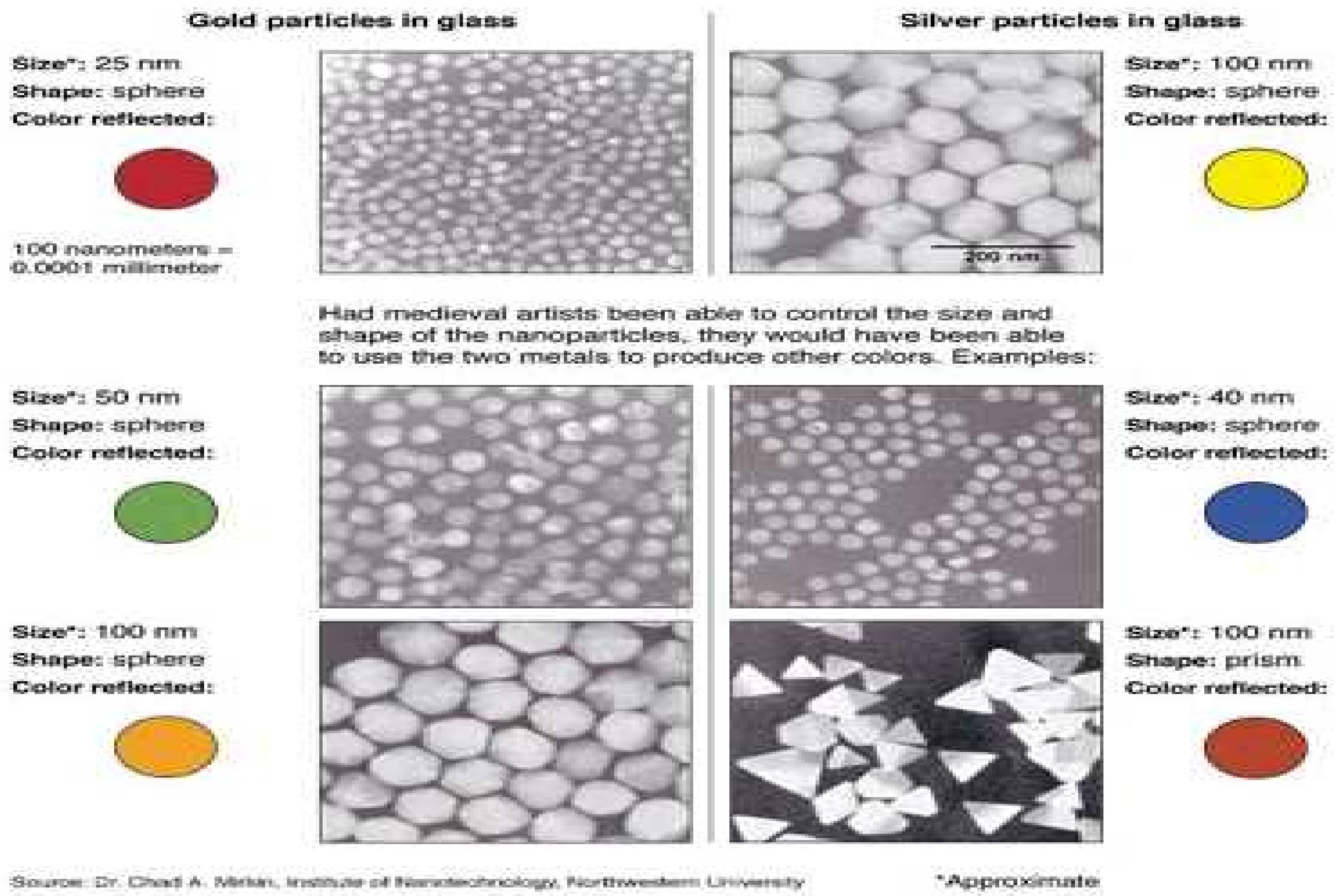


Influece of particle size on Ultimate Strength



Tensile test of Cuprum
Strength 2,3 x greater

Nanoparticle colours



Zdroj obrázku: Institute of Nanotechnology, Northwestern University