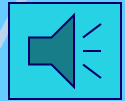


Audio test:



Synergie vlastností jádra a povrchu II



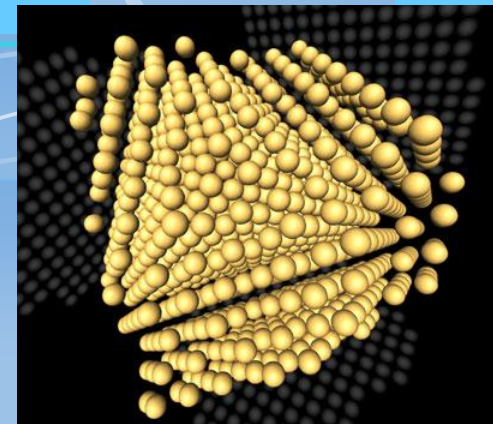
Brno, PS 2012

Start



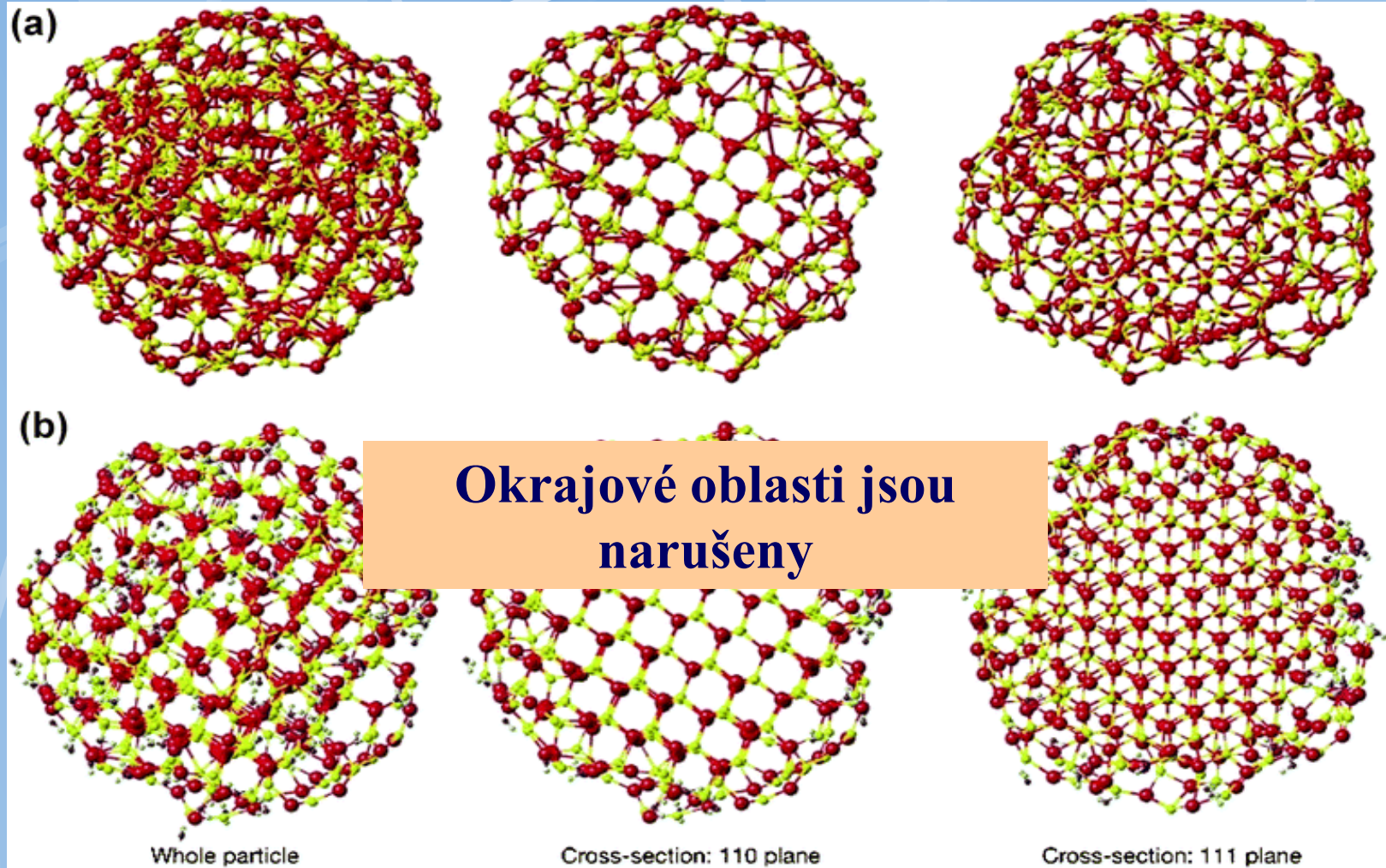
Přednášející: doc. Jiří Sopoušek E-mail:
sopousek@mail.muni.cz, tel.: 549497138

Ofice: UKB A12/M231



Má Au nano volný povrch ?

Stuktura jádra a a povrchu



Simulace ZnS 3nm NPs.

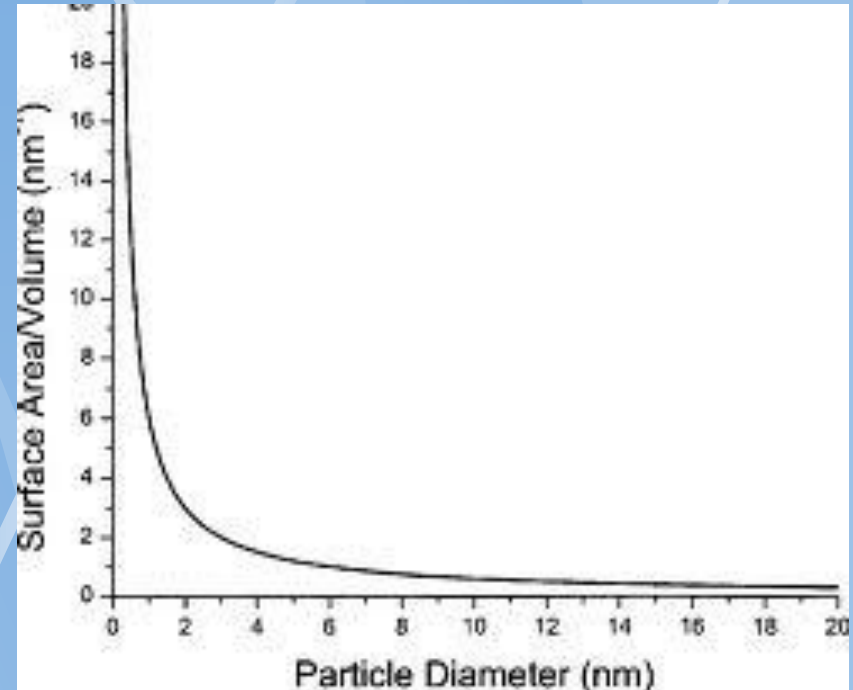
Molecular dynamics prediction of the structure of a “spherical” 3 nm ZnS nanoparticle. (a) Without surface-bound water, and (b) with surface-bound water. S atoms are shown in yellow, Zn atoms are shown in red, O atoms are shown in blue, and H atoms in light blue. The 3-D structures are shown in the left column, and cross-sections through central (110) and (111) planes are shown in the central and right columns, respectively. Reproduced with permission from ref. 103, Nature Publishing Group © 2003.

Synergie vlastností jádra a povrchu

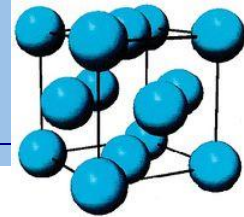
Vlastnosti atomu uvnitř nanočástice jsou ovlivněny povrchovými atomy a naopak.

Corre malý podíl mřížkových defektů

Shell zvýšená povrchová energie, místo anihilace poruch mřížky core.



Závislost mřížkového parametru Au-NPs na velikosti



Výpočet specifické hmotnosti nanočástice

$$\rho = \frac{m}{V} = \frac{M}{V_m}$$

Molární hmotnost.

Molární objem a objem buňky fcc

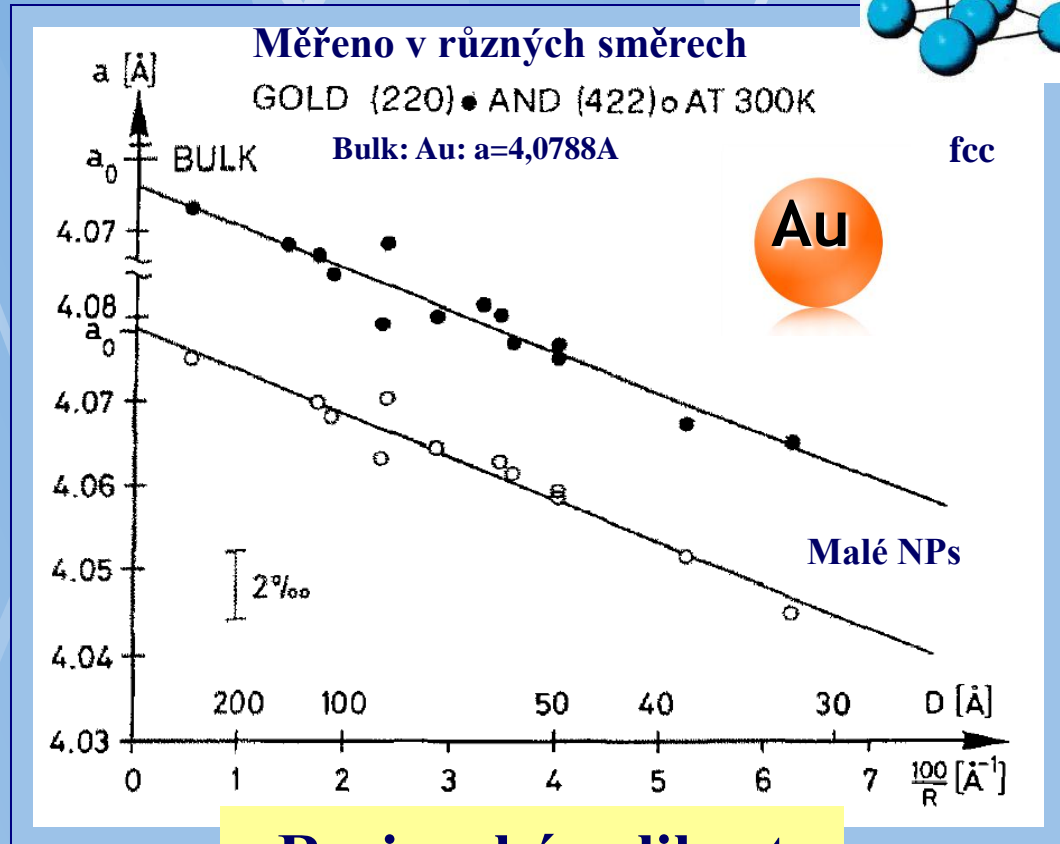
$$V_m = V_{\text{cell}} \frac{N_{\text{Av}}}{N_{\text{cell}}}$$

Avogadrova konst.

$$V_{\text{cell}} = a^3 = \left(2\sqrt{2} \cdot r_{\text{at}}\right)^3, \quad N_{\text{cell}(\text{fcc})} = 4$$

- vakuové napařování na grafitové podložce- kuličky (pro měření V_m)
- TEM (velikost částic) ED (mřížkový parametr)

Molární objem AuNPs není shodný s bulkem. NPs mají menší základní buňku.

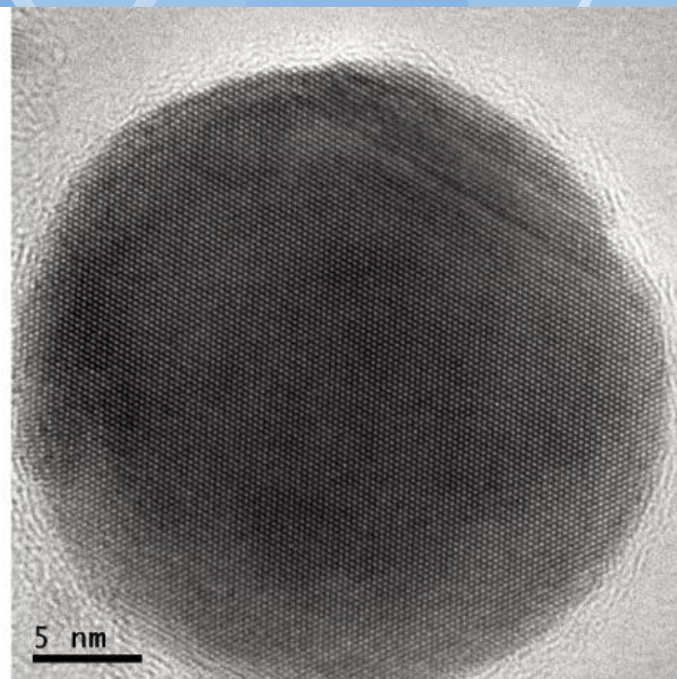
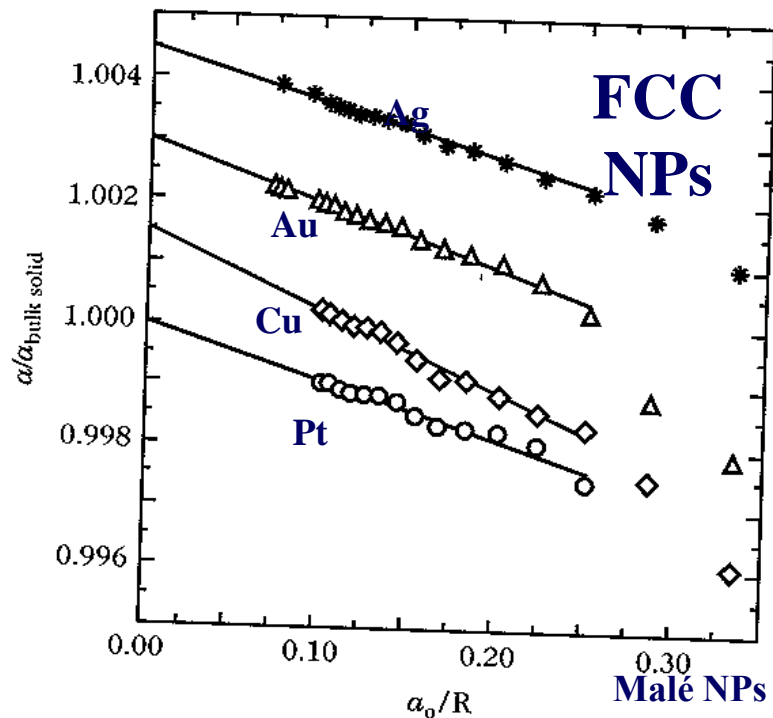


SURFACE STRESS AND SIZE EFFECT ON THE LATTICE PARAMETER IN SMALL PARTICLES OF GOLD AND PLATINUM

C. SOLLIARD and M. FLUELI

Surface Science 156 (1985) 487-494
North-Holland, Amsterdam

Změna parametrů mřížky



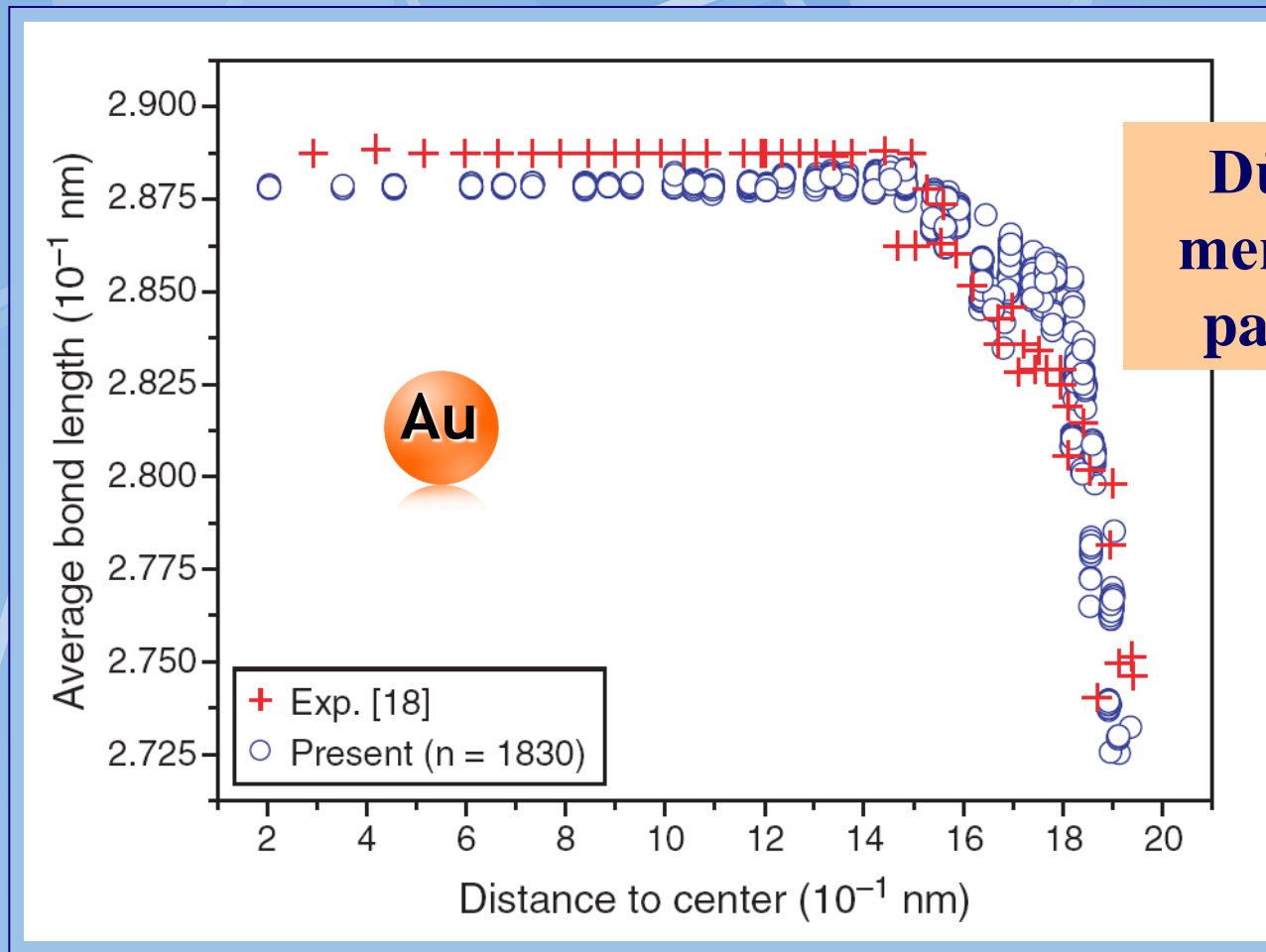
Závislost změny fcc mřížkového parametru NPs (vůči bulk Pt) na reciproké velikosti nanočástic Ag, Au, Pt (obtížně měřitelné ale zřetelné trendy).

Silver nanoparticles. Overview (left, TEM) and detail (right, HRTEM).
Silver fcc lattice

($a=0.424\text{nm}$, tabulated value for Ag:
 $a_0=0.40862\text{nm}$).

$\{a_0/r=0.40862\text{nm}/30\text{nm}=0,0146\text{nm}^{-1}$
 $\frac{1}{2} \frac{a}{a_0}=1.038\}$..nesoulad 10x

Povrchová komprese vazeb



**Důsledkém je
menší mřížkový
parametr NPs**

$$r_{\text{np}} = r_{\text{Au}} \left(\frac{N_{\text{Au}}}{f_{\text{fcc}}} \right)^{1/3} = 0,144 \left(\frac{1830}{0,74} \right)^{1/3} = 1,95 \text{ nm}$$

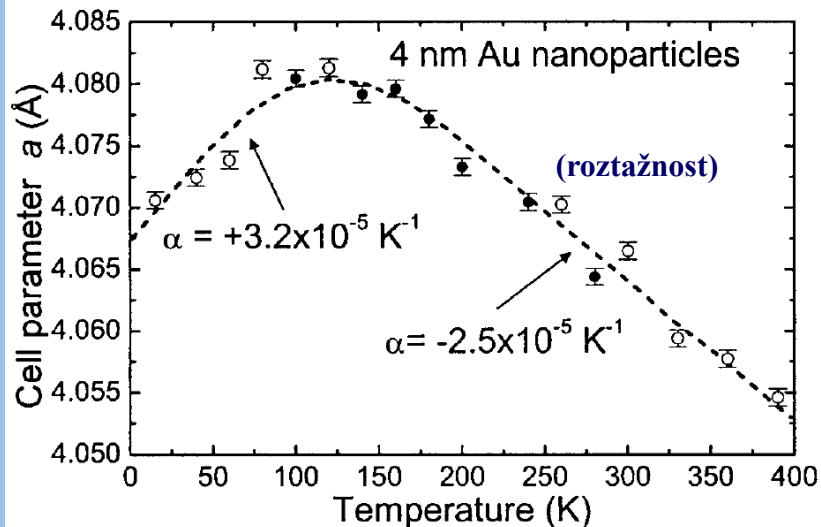
Bond-Length and -Energy Variation of Small Gold Nanoparticles

Weihong Qi^{1,2,*}, Baiyun Huang^{1,3}, and Mingpu Wang^{1,2}

*Journal of
Computational and Theoretical Nanoscience*
Vol. 6, 635–639, 2009

Vliv teploty na mřížkový parametr nečekané tendence

Au: za nízkých a vysokých teplot je mřížka NPs menší



VOLUME 89, NUMBER 13

PHYSICAL REVIEW LETTERS

23 SEPTEMBER 2002

Thermal Contraction of Au Nanoparticles

W.-H. Li, S. Y. Wu, C. C. Yang, S. K. Lai, and K. C. Lee

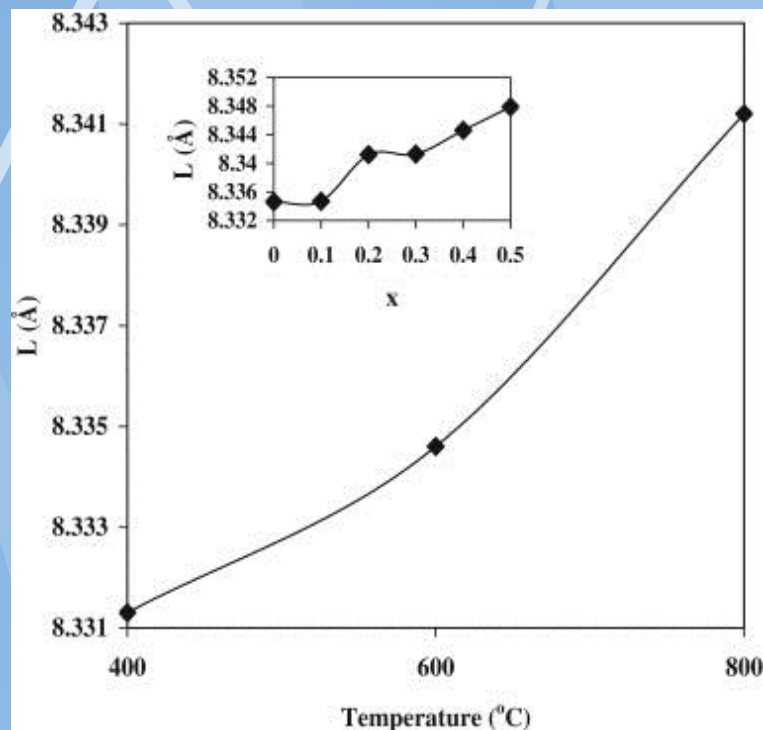
Department of Physics, National Central University, Chung-Li, Taiwan 32054, Republic of China

H. L. Huang and H. D. Yang

Department of Physics, National Sun Yat-Sen University, Kaohsiung, Taiwan 804, Republic of China

(Received 17 April 2002; published 5 September 2002)

Ni_{0.5}Li_{0.2}Cu_{0.4}Fe₂O₄ ferrites: nejasná pravidla

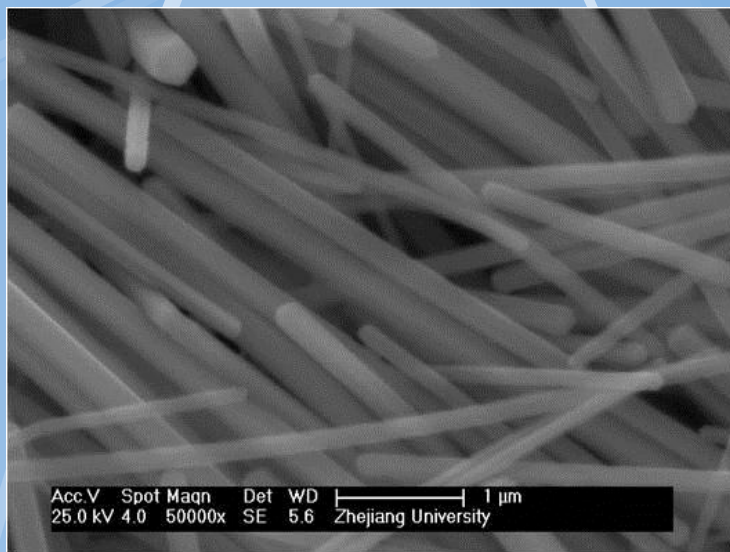


Temperature dependence of lattice constant (L) for $\text{Ni}_{0.5}\text{Li}_{0.2}\text{Cu}_{0.4}\text{Fe}_2\text{O}_4$ ferrites. Inset: composition dependence of lattice constant (L) for $\text{Ni}_{0.5}\text{Li}_{1.0-2x}\text{Cu}_x\text{Fe}_2\text{O}_4$ ferrites at $T_a=600^\circ\text{C}$.

<http://www.sciencedirect.com/science/article/pii/S0304885310007080>

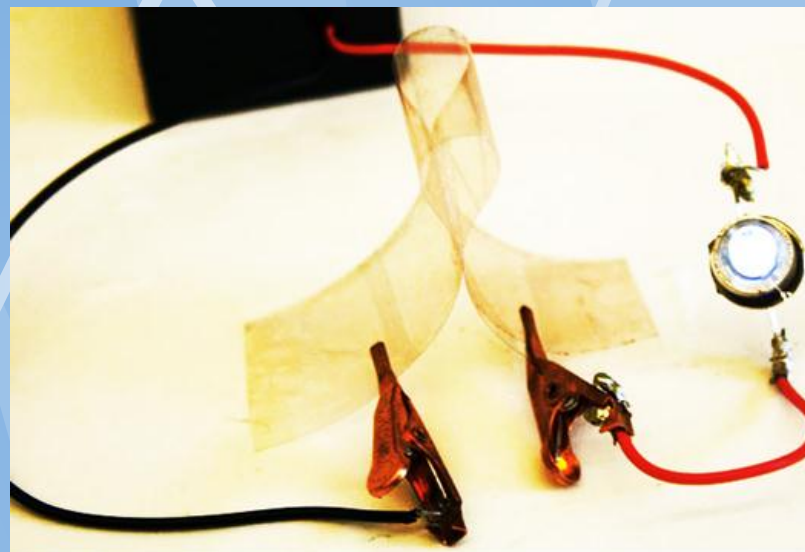
Elektrická vodivost NPs

Hlavní reprezentanti: nanovlákná na bázi kovů ale i anorganických látek (nanowires – NWs), nanokompozity, uhlíková nanovlákná (CNTs).



Silver Nanowires
AWS180(D=150-210nm), komerční produkt (<http://www.ke-chuang.com/productshow.asp?id=71>)

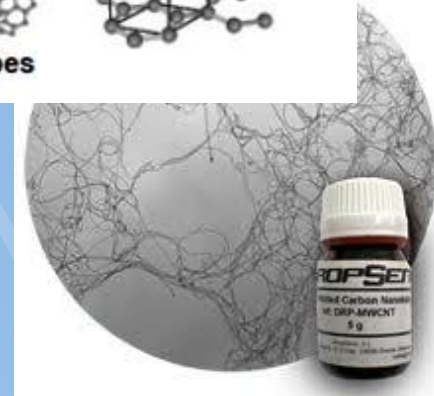
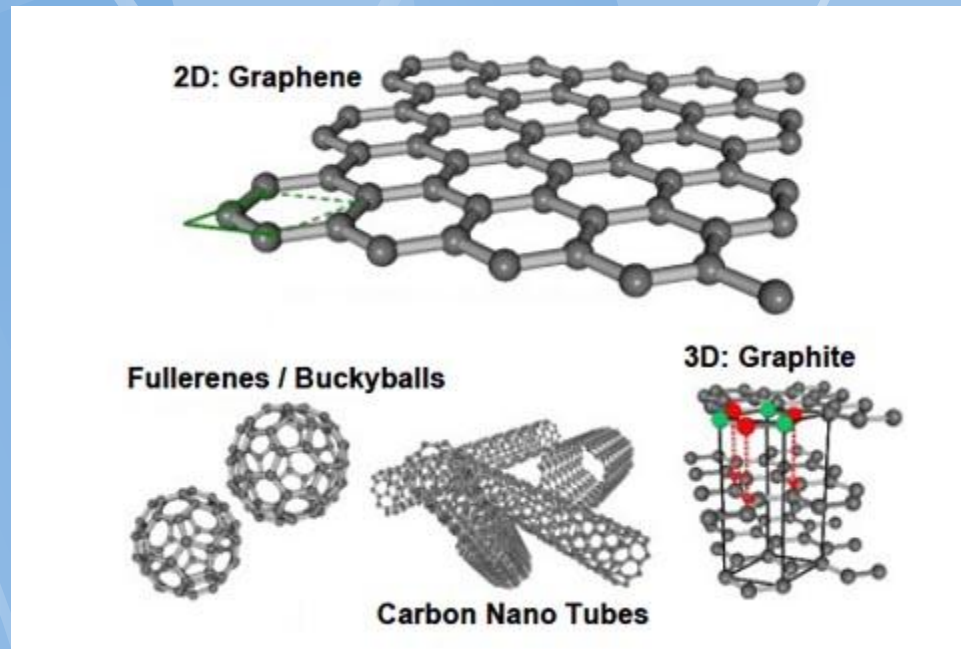
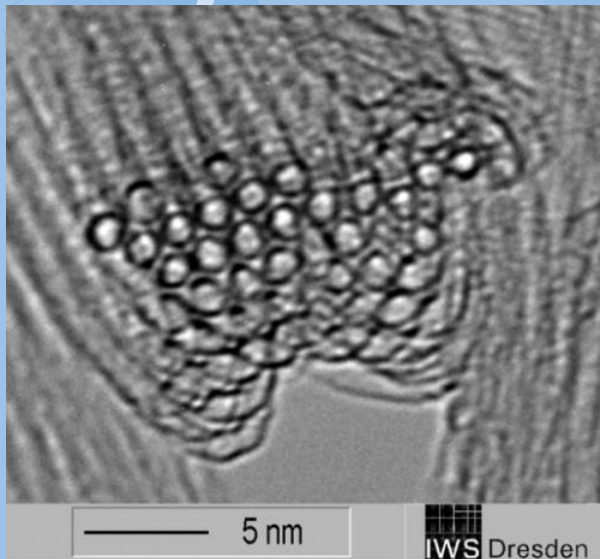
Elektrická vodivost NPs úzce a úměrně souvisí s tepelnou vodivostí.



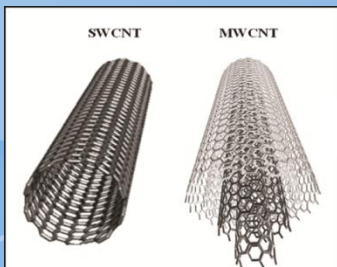
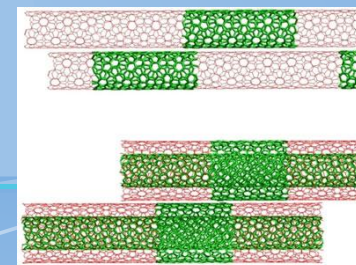
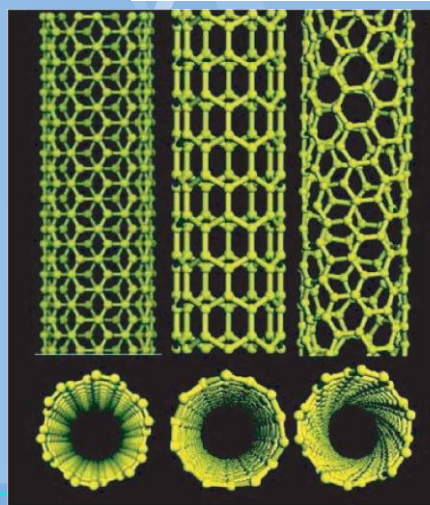
A new flexible film made of copper nanowires and plastic conducts electricity illuminating a small light bulb. (Credit: Ben Wiley, Duke University). <http://www.futurity.org/science-technology/cheaper-touch-screens-from-copper-film/>

Carbon Nanotubes (CNTs)

Vodivost se blíží kovům a polovodičům.
Problém s délkou, vzájemnými
propojeními a manipulací i klasickým
měřením vodivosti.

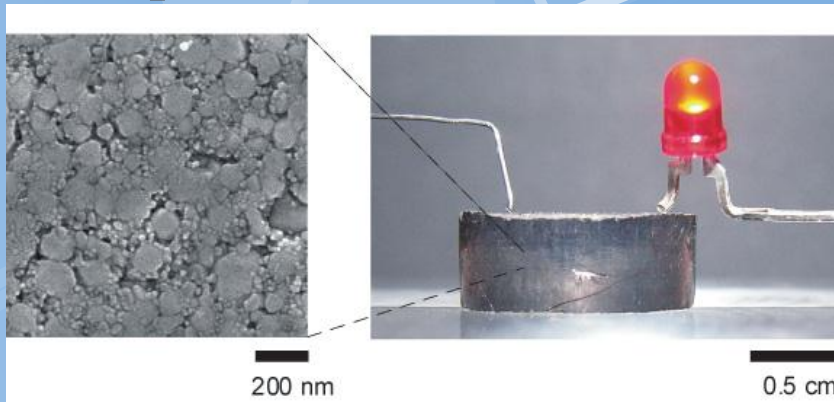


<http://www.printedelectronicsworld.com/articles/production-of-low-defect-single-walled-carbon-nanotubes-00004439.asp>



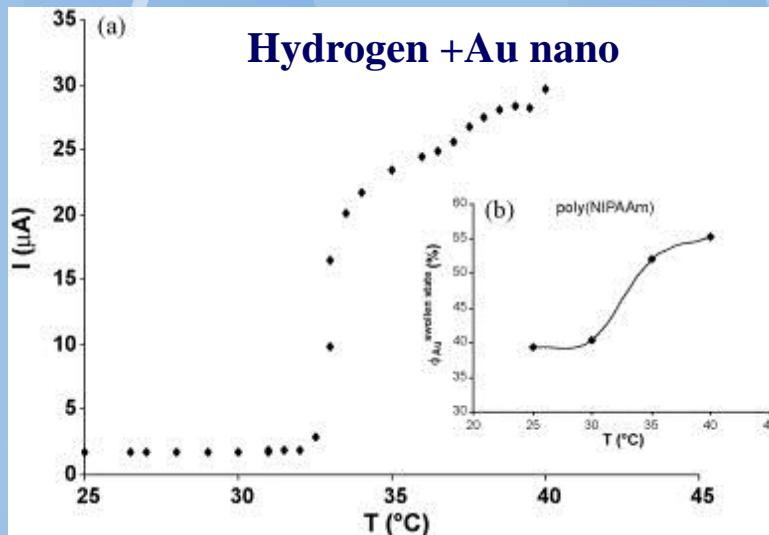
MultiWall
CNTs
MWCNTs

Elektrická vodivost souboru NPs závisí především na vlastnostech povrchu

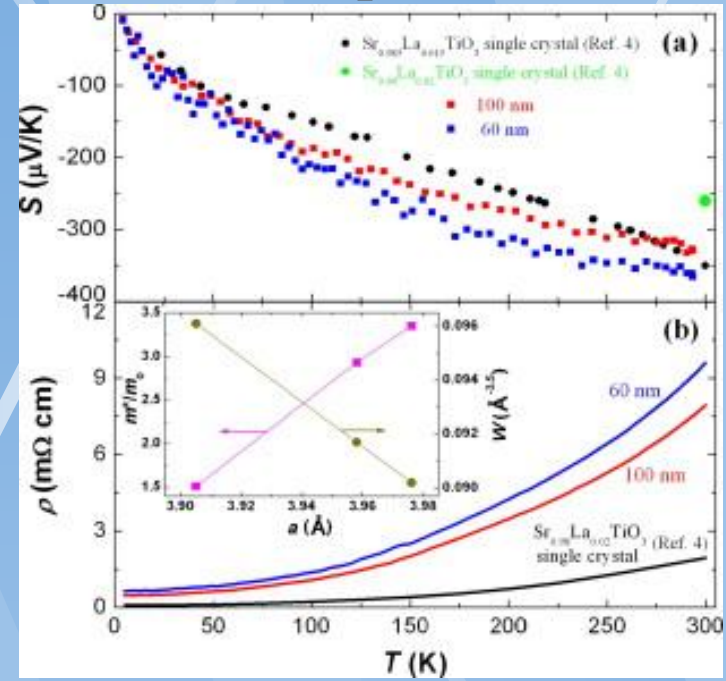


Flame synthesis CoNb nanocomposit:

http://www.fml.ethz.ch/research/Former_researchprojects/nonoxidenanoparticles



<http://www.sciencedirect.com/science/article/pii/S0169433209016213>



Temperature dependences of (a) thermopower S and (b) resistivity ρ for the nanoparticle compacts and single crystals. The data of the single crystals are from Ref. [4]. The inset of (b) presents the variations of effective mass m^* and bandwidth W as a function of the lattice parameter a .

<http://www.sciencedirect.com/science/article/pii/S1359646211001692>

Vodivost Ag-nano

Diskuse



● Zjistit co dělají na pensylvánské Univ.:

- El. články s nano: <http://inhabitat.com/researchers-shine-light-on-gold-nanoparticles-to-produce-electricity/>

