The influence of chromium on thermal evolution of stabilized zirconia nanoparticles and their surface state

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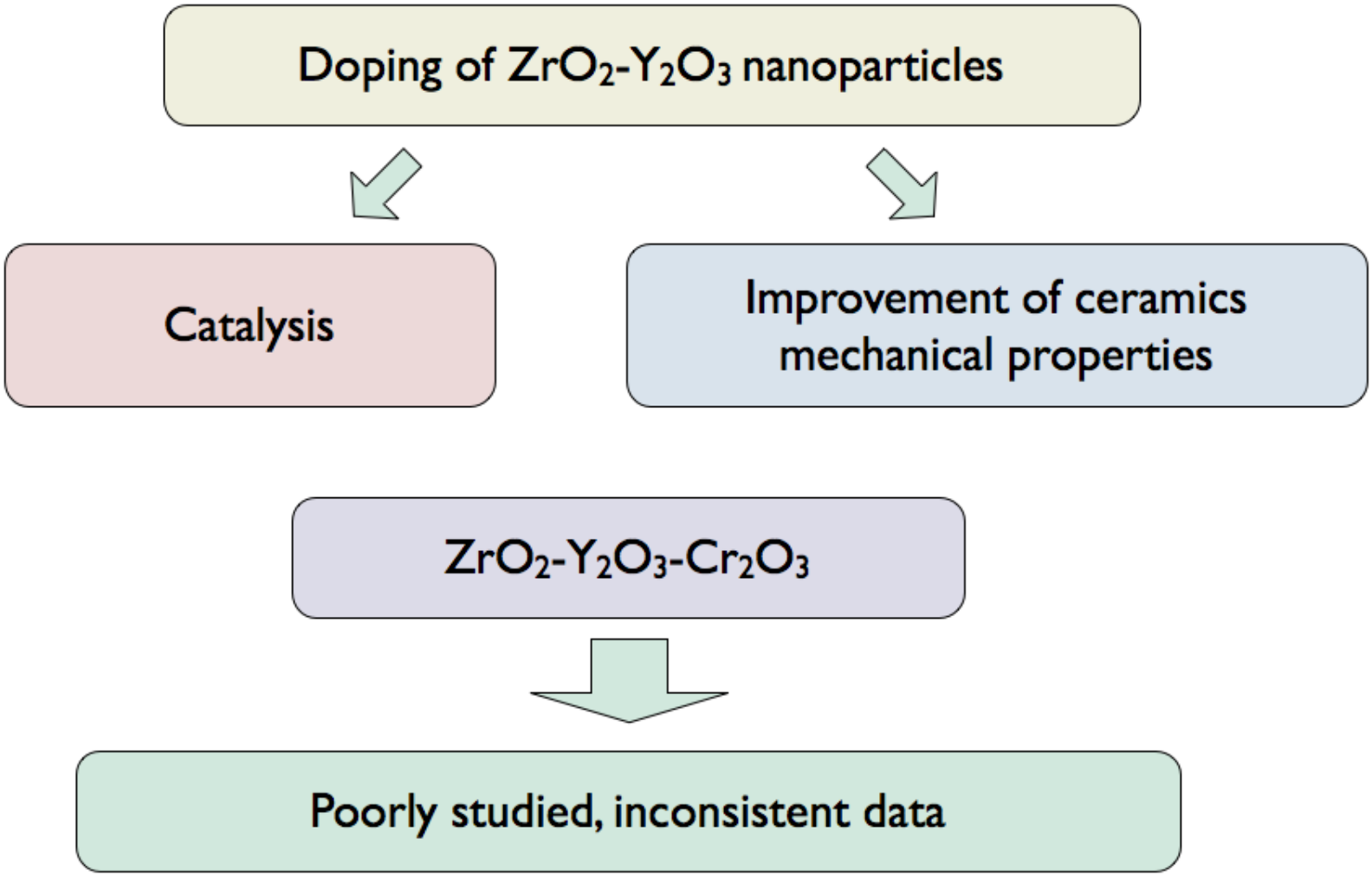
Doping of ZrO_2

Stabilizer: Y, Ca, Mg	Modifying addition Al, Fe, Cr	Multicomponent doping ZrO_2-Y_2O_3-Cr_2O_3
Expanded temperature range of application	Mechanical properties Electrical properties Catalytic activity	Material with improved/new properties working in wide temperature range

Motivation


Doping of ZrO_2-Y_2O_3 nanoparticles
Catalysis
Improvement of ceramics mechanical properties
ZrO_2-Y_2O_3-Cr_2O_3
Poorly studied, inconsistent data

Materials & methods

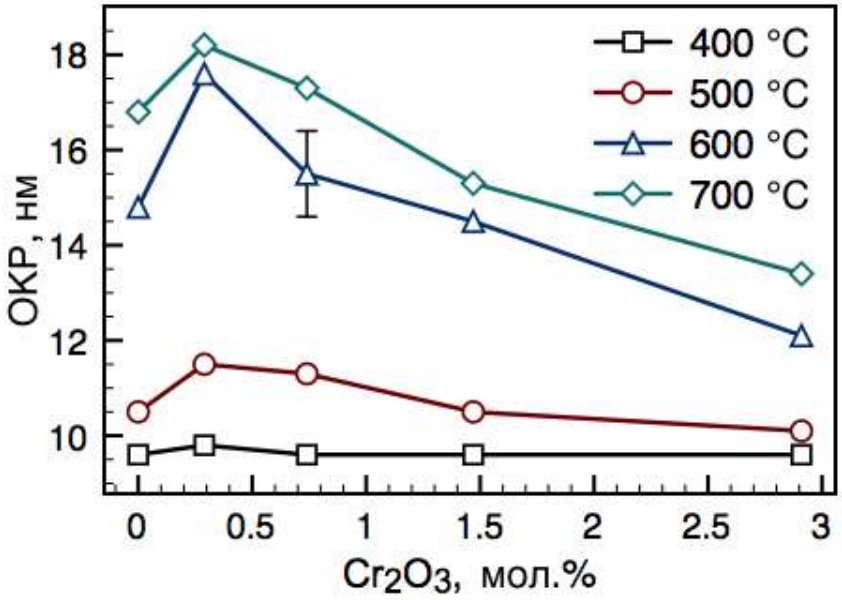
Nanopowders of zirconia dioxide are synthesized by co-precipitation technique developed in materials science department of DonPhTI

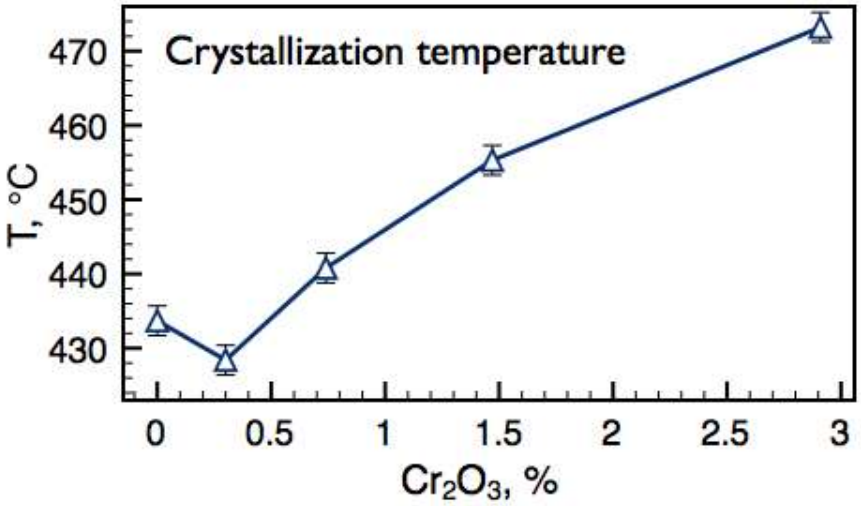
Label	Chemical composition
Z3Y	ZrO_2+3 mol.% Y_2O_3
Z3Y0.3Cr	ZrO_2+3 mol.% Y_2O_3 + 0.3 % Cr_2O_3
Z3Y0.75Cr	ZrO_2+3 mol.% Y_2O_3 + 0.75 % Cr_2O_3
Z3Y1.5Cr	ZrO_2+3 mol.% Y_2O_3 + 1.5 % Cr_2O_3
Z3Y3.0Cr	ZrO_2+3 mol.% Y_2O_3 + 3.0 % Cr_2O_3

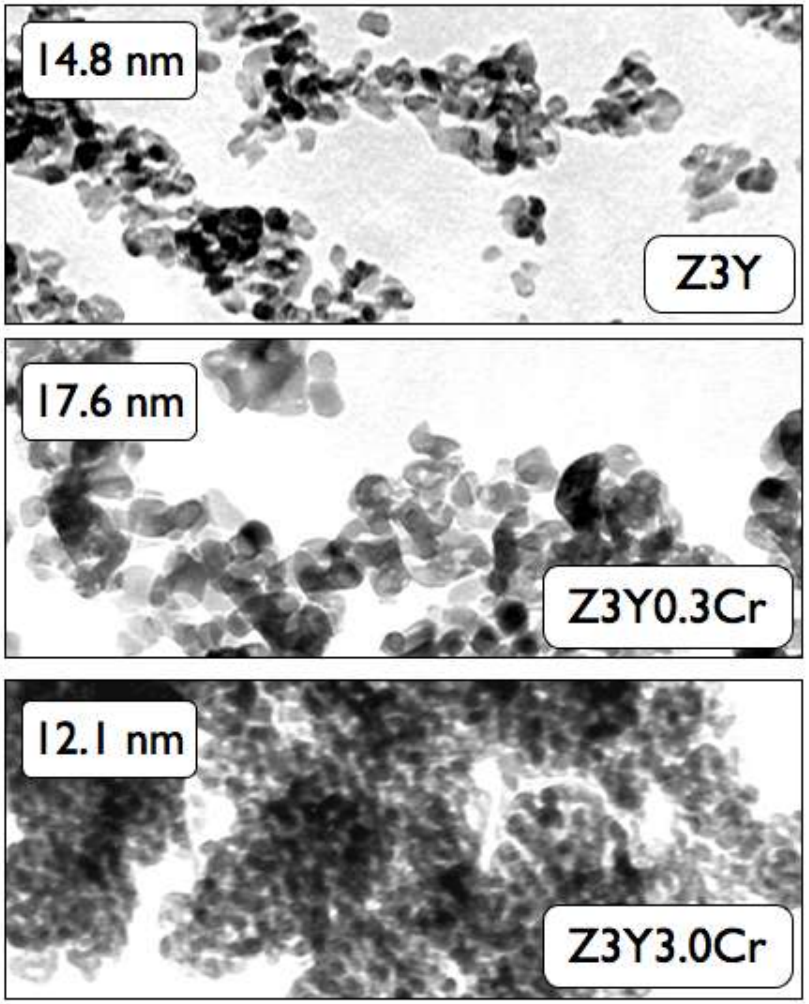
Methods

- X-ray Photoelectron spectroscopy
- ESR spectroscopy
- NMR spectroscopy
- FTIR spectroscopy
- X-ray diffraction
- TG & DSC analysis
- SEM & TEM analysis
- BET specific surface

Size dependence on chromium concentration

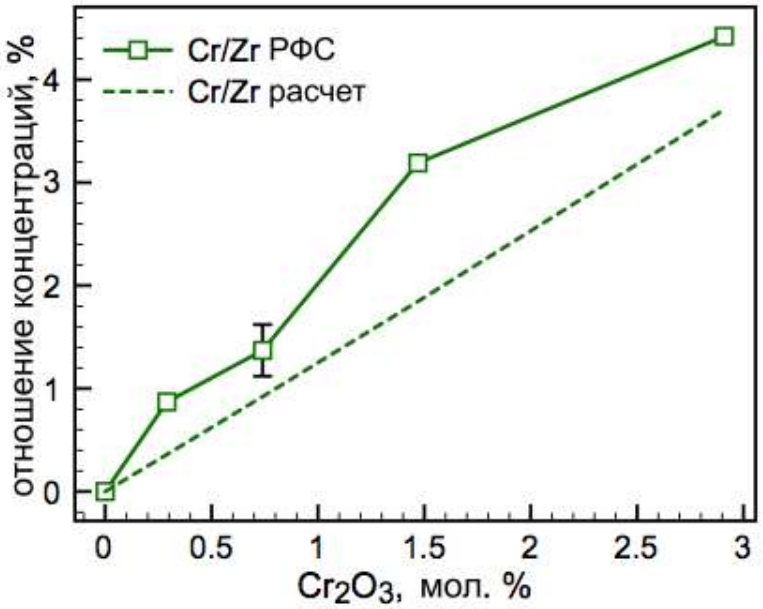


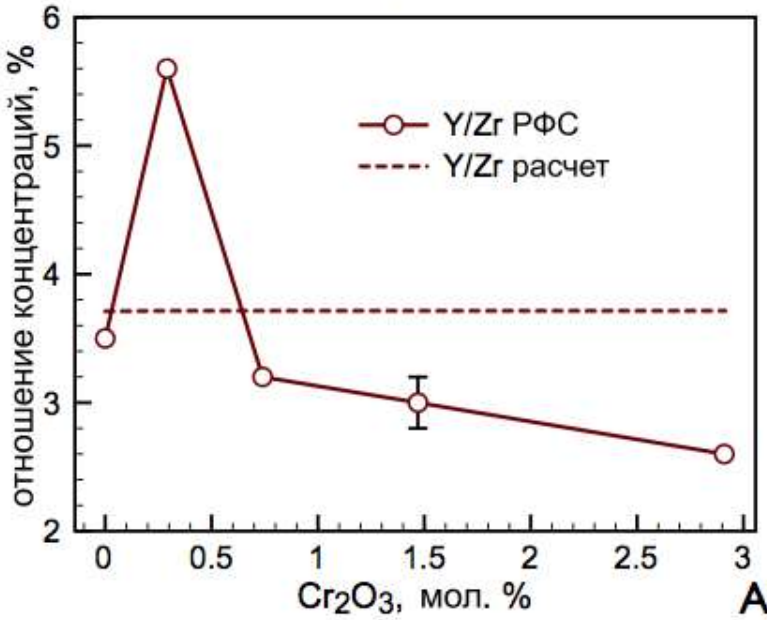


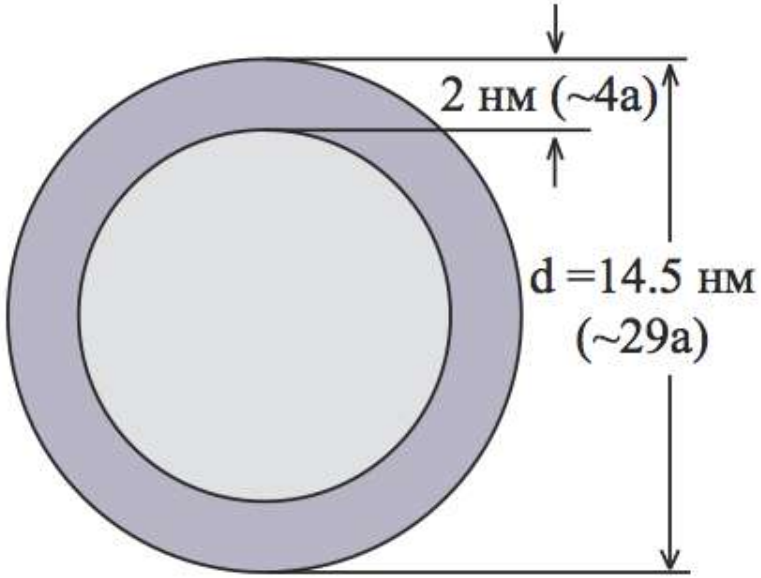


T_c = 600 °C

Y & Cr on the surface of the nanoparticles







$N_S = 18180$; $N_V = 24389$; a = 5.10 Å

$$D(T) = D_0 e^{-\frac{E_a}{kT}}$$

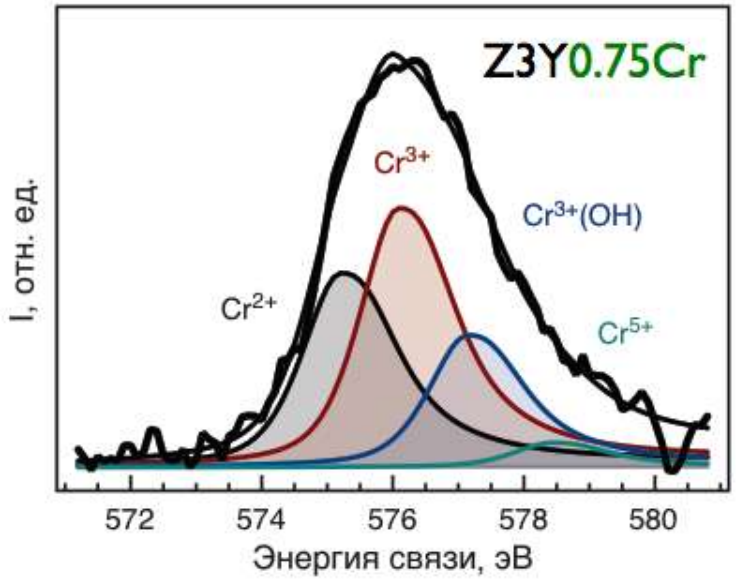
T_c = 600°C

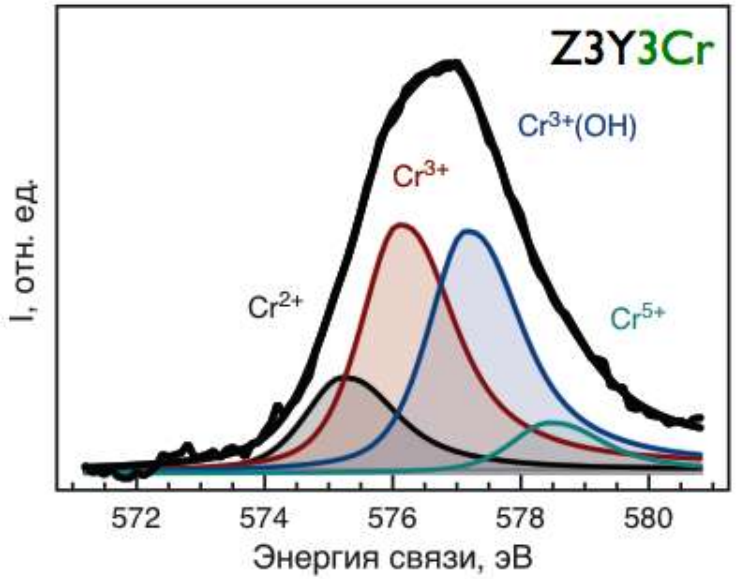
t_c = 2 h

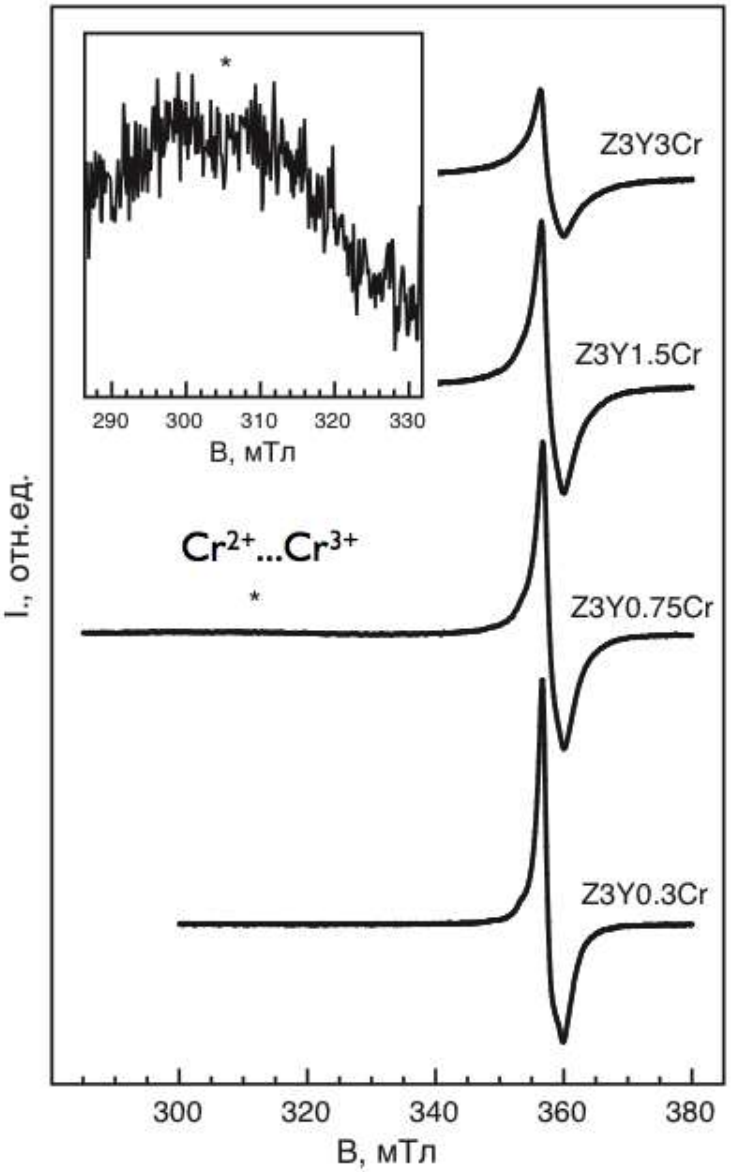
$$\left.\begin{aligned} l_{Zr} &= 9.1 \cdot 10^{-6}\, nm \\ l_Y &= 1.4 \cdot 10^{-4}\, nm \\ l_{Cr} &= 0.65 nm \end{aligned}\right\} \ll \frac{d}{2} - 4a$$

Applied Surface Science, 256, (2010), pp. 7175–7177

Cr charge states. XPS, ESR

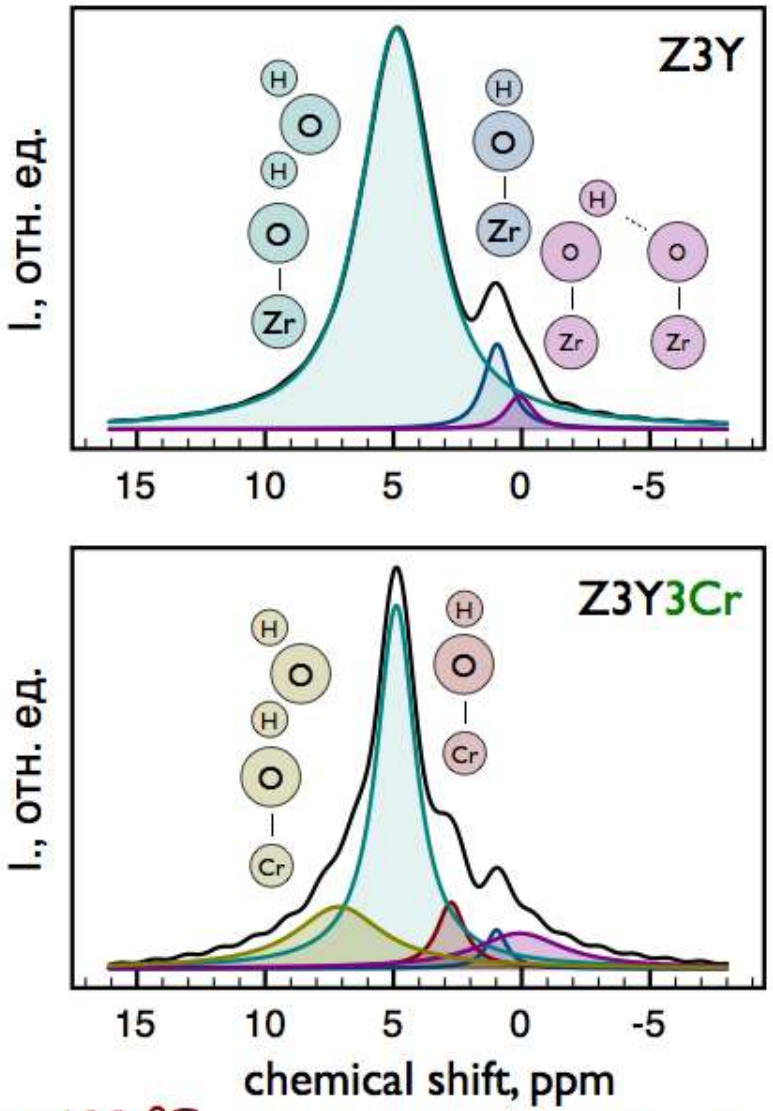


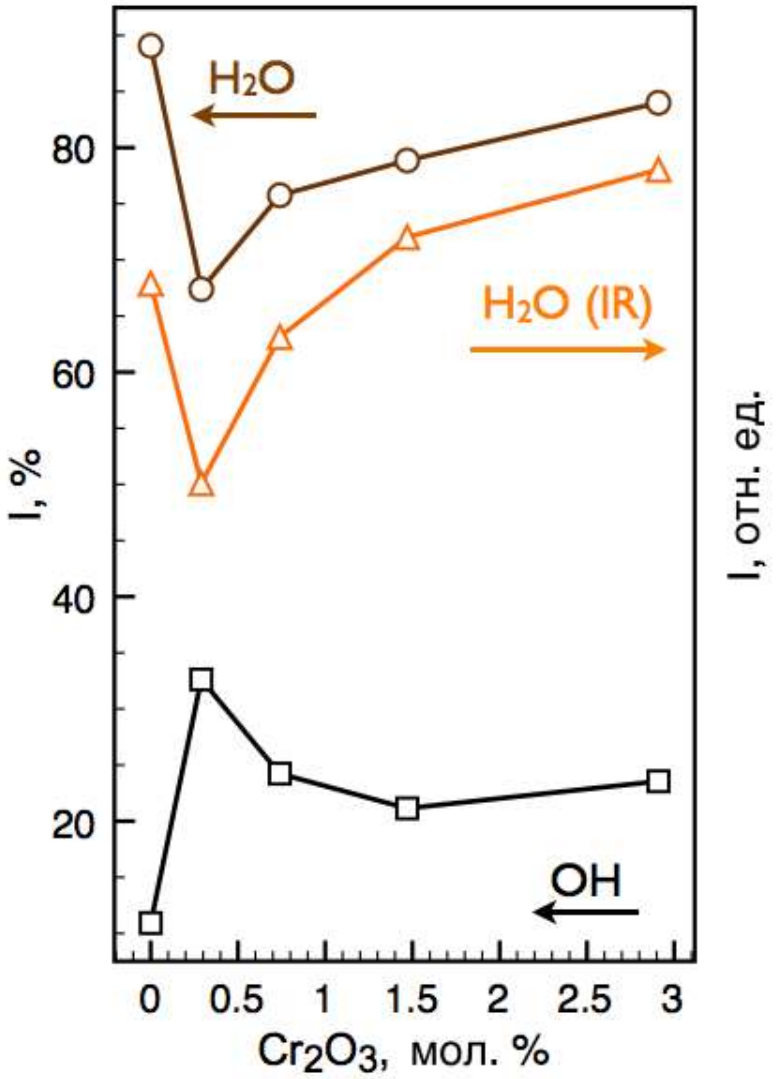




Functional Materials, 17 [3], pp. 306-310, (2010)

Hydrous shell structure. NMR, FTIR

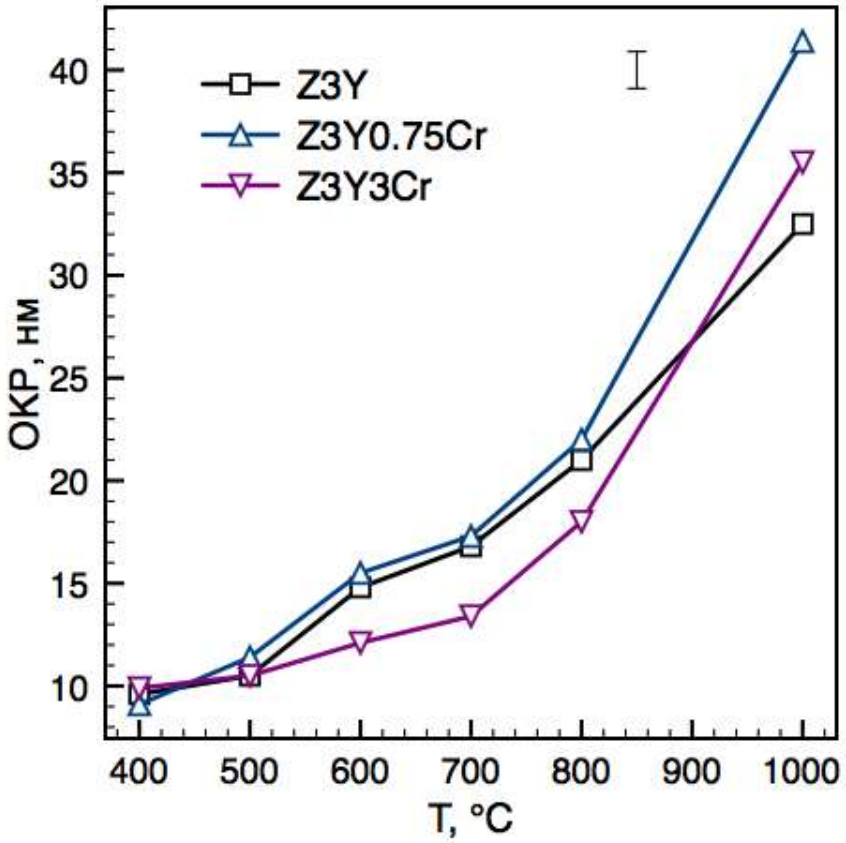




T_c = 600 °C

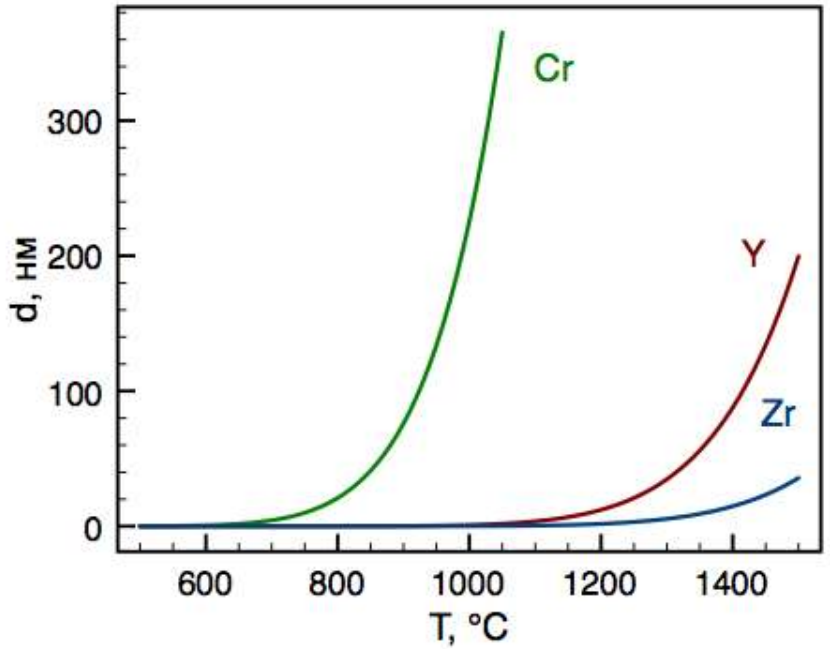
Physics and chemistry of solid state, 11[1] (2010) pp. 181-184

Growth rate of zirconia nanoparticles doped with chromium

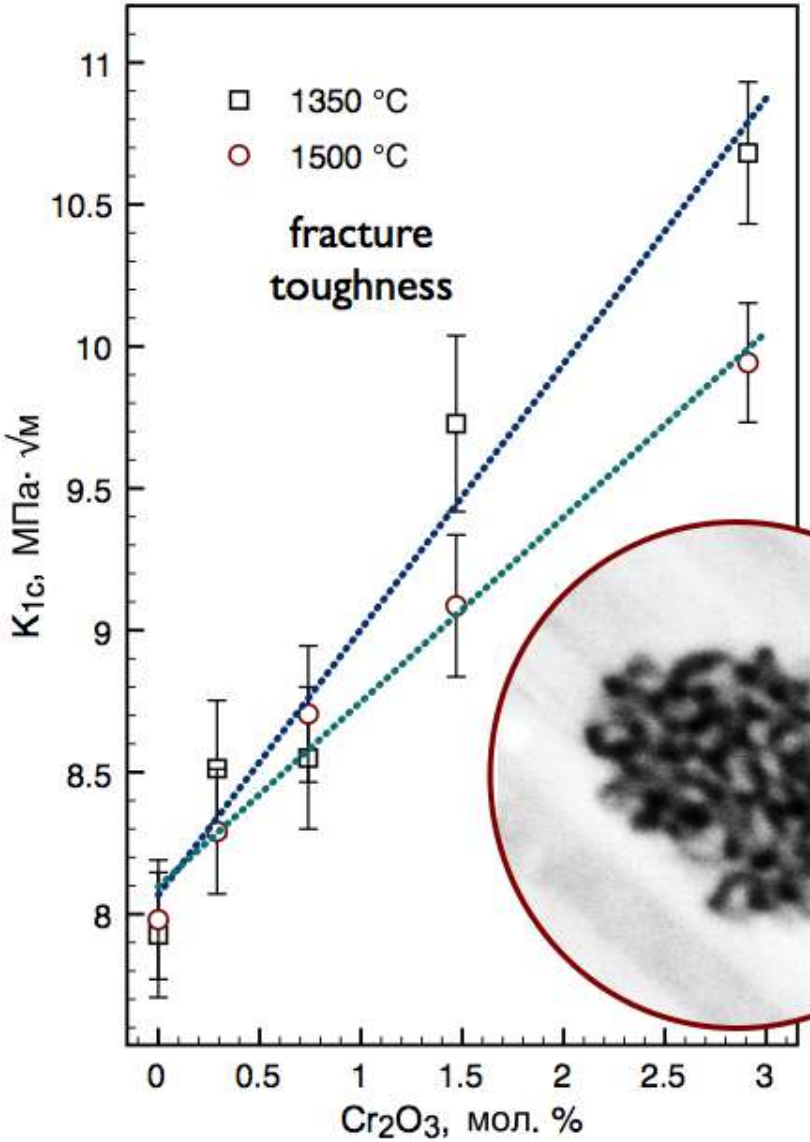


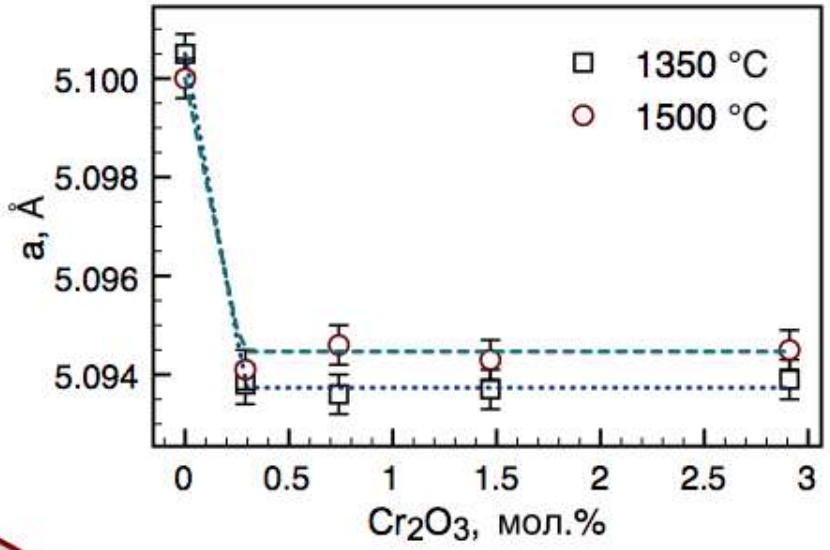
$$D(T) = D_0 e^{-\frac{E_a}{kT}}$$

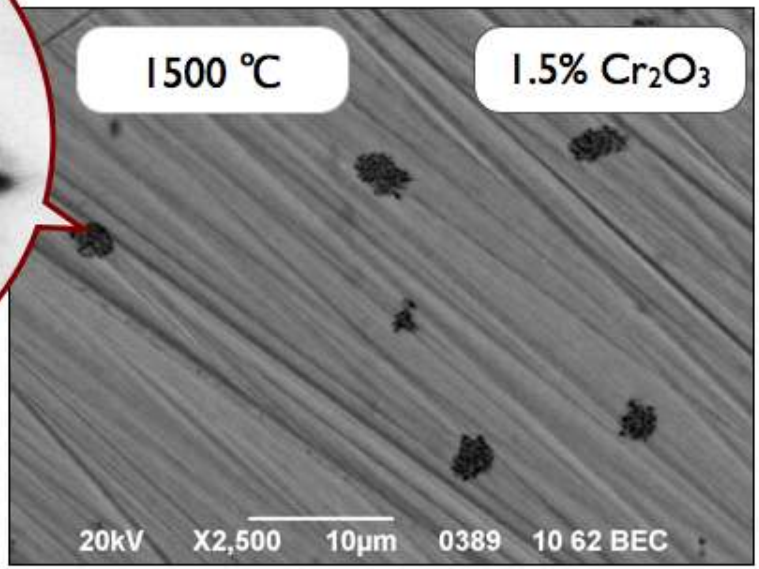
	E_a, эВ
Cr	2.7
Y	4.2
Zr	4.5



Composite zirconia ceramics

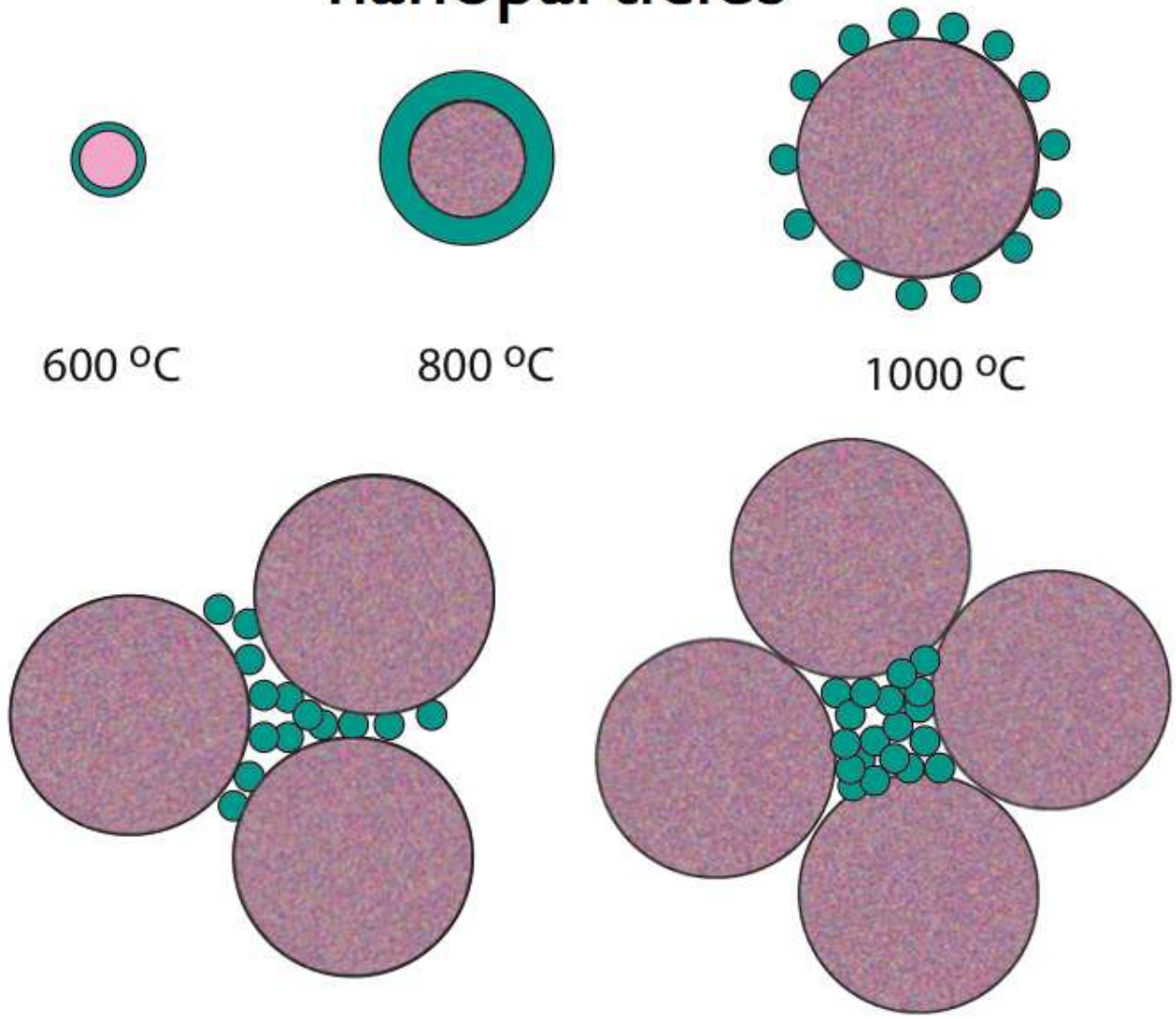


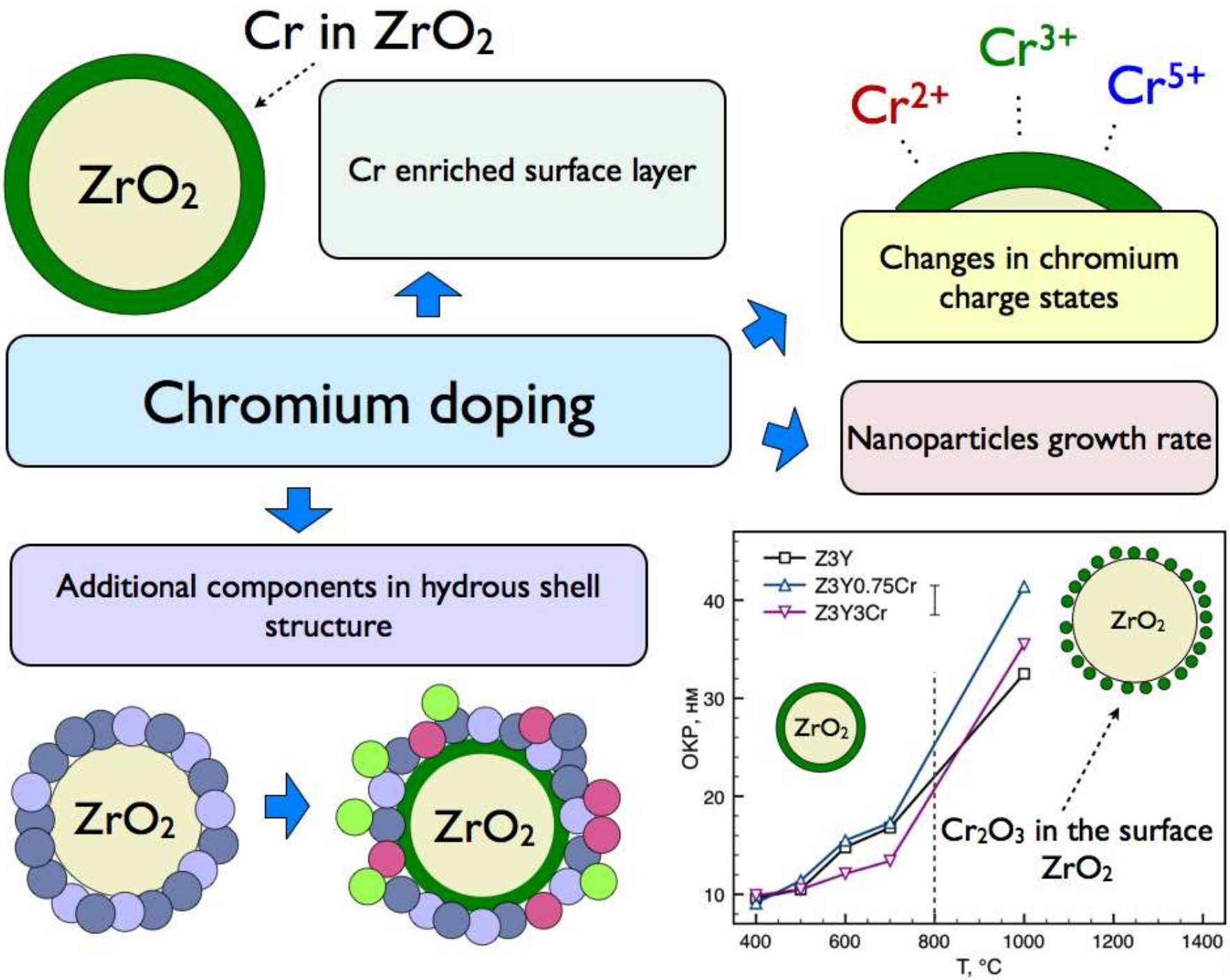




Nanostructural materials science №2, p. 51-57 (2010)

Consolidation of chromium enriched nanoparticles




Cr in ZrO_2
ZrO_2
Cr enriched surface layer
Cr^{2+}
Cr^{3+}
Cr^{5+}
Changes in chromium charge states
Chromium doping
Nanoparticles growth rate
Additional components in hydrous shell structure
ZrO_2
ZrO_2
Z3Y
Z3Y0.75Cr
Z3Y3Cr
OKP, нм
40
30
20
10
400
600
800
1000
1200
1400
T, °C
ZrO_2
ZrO_2
Cr_2O_3 in the surface ZrO_2

Thank You for Your attention!