TSE theories comparison

1. Pawlow's result (first order TD, fTD)

$$\frac{T-T_0}{T_0}=\left.\frac{\Delta T}{T_0}\right|_{fTD}=-\frac{2}{LR\rho_S}\left(\gamma_S-\gamma_L\left(\frac{\rho_S}{\rho_L}\right)^{2/3}\right)=-\frac{A}{R}<0$$

2. Liquid Layer Model (LLM)

$$\left.\frac{\Delta T}{T_0}\right|_{LLM}=-\frac{2\gamma_{SL}}{\rho_S L(R-\delta)}-\frac{2\gamma_{LV}}{\rho_S LR}\left(1-\frac{\rho_S}{\rho_L}\right)=-\frac{A}{R-\delta}-\frac{B}{R}$$

3. Smooth interfaces interaction (SII)

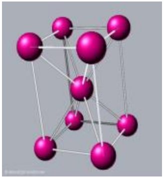
$$\left.\frac{\Delta T}{T_0}\right|_{SII}=-\frac{2\gamma_{SL}}{\rho_S L(R-\delta)}\left(1-e^{-\delta/\xi}\right)-\frac{\Gamma R^2}{\rho_S L\xi(R-\delta)^2}e^{-\delta/\xi}=-\frac{A}{R-\delta}\left(1-e^{-\delta/\xi}\right)-\frac{B\Gamma R^2}{(R-\delta)^2}e^{-\delta/\xi}$$

4. Thermal expansion variation (TEV)

$$\left.\frac{\Delta T}{T_0}\right|_{TEV}=-\frac{2}{\rho_S RL}\left(\gamma_{SM}-\gamma_{LM}\left(\frac{\rho_S}{\rho_L}\right)^{2/3}\right)+\frac{\Delta E}{L}$$

ΔE = strain energy difference (thermal expansion matrix-cluster)

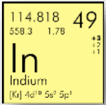
TSE in In NCs in silica

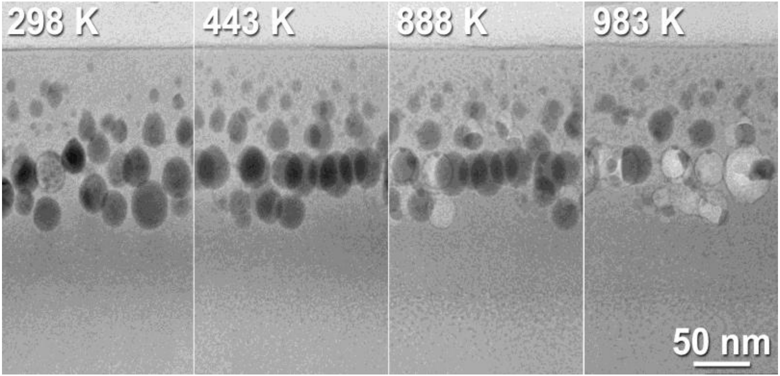


In = tetragonal cell

T_M (bulk) = 429.8 K
(156.6 °C)

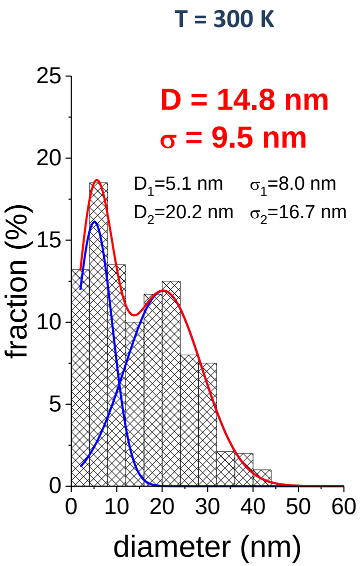
In^{2+} implantation in silica
Energy: 320 keV
Fluence: 2×10^{17} In^{2+}/cm^2
Rp = 100nm (ion projected range)
ΔRp=70nm (straggling)

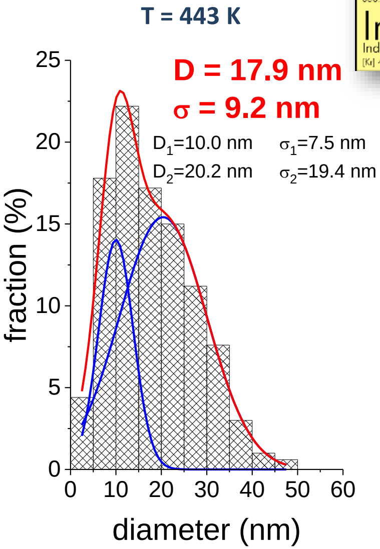


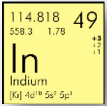


M. A. Tagliente, G. Mattei, L. Tapfer, M. Vittori Antisari, and P. Mazzoldi, Phys. Rev. B 70 (2004) 075418

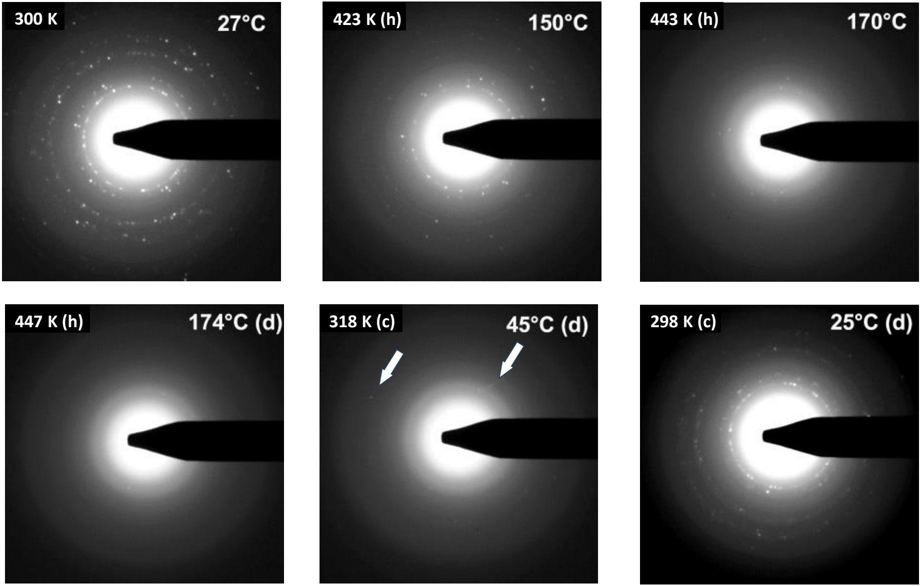
TSE in In NCs in silica





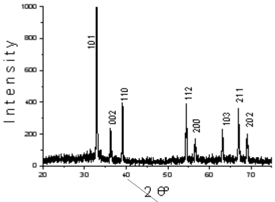


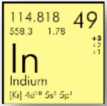
TSE in In NCs in silica

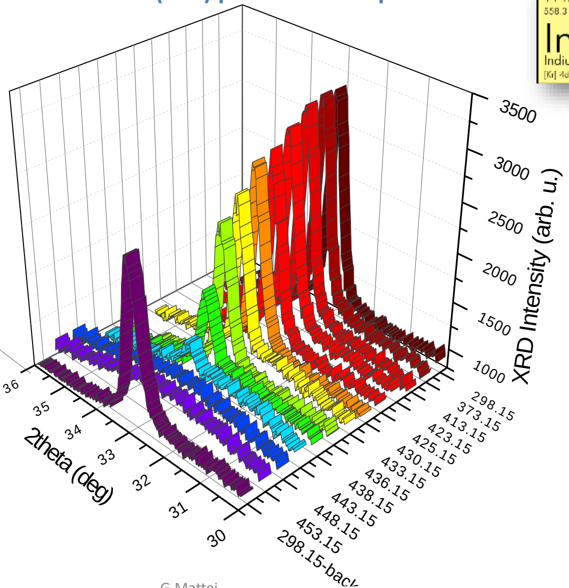


TSE in In NCs in silica

GIXRD evolution of the In (101) peak with temperature

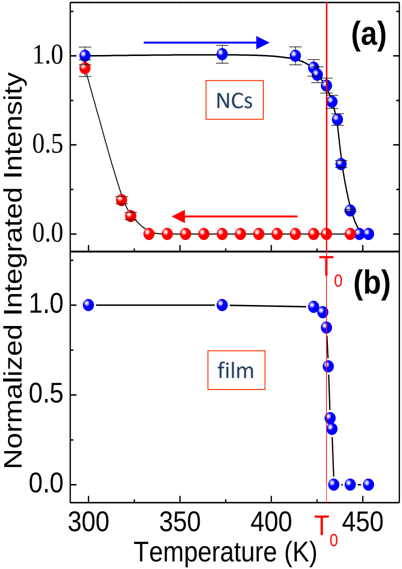






TSE in In NCs in silica

GIXRD analysis



(a) Normalized integrated intensity of the nanoclusters In (101) GIXRD peak versus the temperature for the thermal cycle between RT and 453 K. Blue and red solid circles represent data obtained during the heating and cooling sequences, respectively. T_0 indicates the In bulk melting point (430 K)

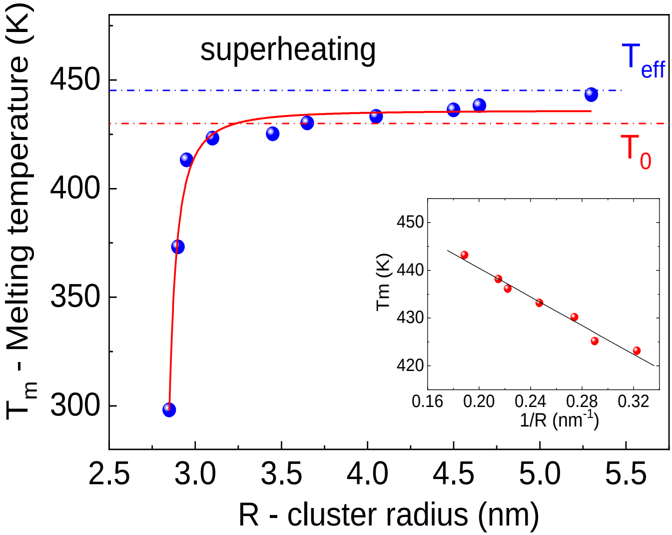
(b) Normalized integrated intensity of a In film evaporated on a glass substrate. T_0 indicates the In bulk melting point.

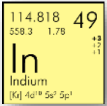
Thermal hysteresis loop for In NCs in SiO_2:

Superheating of 13±1 K

Supercooling of 107±1 K

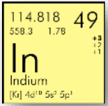
TSE in In NCs in silica





TSE in In NCs in silica

Some basic thermodynamics…



Pressure on In NCs?

$$K \equiv -\frac{1}{V}\frac{\partial V}{\partial P}\bigg|_T$$

$$\Delta P = -\frac{\Delta V}{K\,V} = -\frac{3}{K}\frac{\Delta d}{d}$$

$$\frac{\Delta d_{(101)}}{d_{(101)}}\bigg|_{XRD} = 1.5 \cdot 10^{-3}$$

K = 0.00273 GPa^{-1} (*bulk isothermal compressibility*)

ΔP = 0.17 GPa

Clausius-Clapeyron (*from Gibbs-Duhem*):

$$\frac{dP}{dT} = \frac{L_{mol}}{T_0 \Delta V_{mol}} \qquad \Delta T = \frac{\Delta P}{L} T_0 \Delta V_{mol}$$

L_{mol} = 3.25 kJ/mol

ΔV_{mol} = 0.32 cm^3/mol

ΔP = 0.17 GPa

T_0 = 430 K

ΔT_{theo} ~ 7 K

ΔT_{exp} ~ 13 K