Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Chemical ordering phenomena in nanostructured FePt: Monte Carlo Simulations

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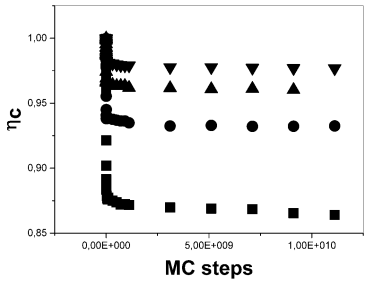
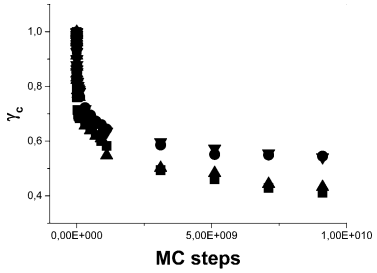
The information presented herein is related to the article published in Physical Chemistry Chemical Physics (doi:…) in the following referred to as "article".

The graphs displayed in Fig.1 illustrate that while after 10^{10} MC steps the inner parts of the samples showed equilibrium atomic configurations, this was not the case of their PD-thick surface-affected parts. The c-$L1_0$ variant LRO parameter η_C and the volume fraction of the c-$L1_0$ variant domains γ_C are defined in the article by Eq.2 and Eq.3, respectively. The particular η_C and γ_C isotherms correspond to reduced temperatures T/T_T where T_T =1575 K denotes the order-disorder $L1_0 \rightarrow A1$ transition temperature simulated for the bulk FePt.

	Inner part	Surface-affected part
nanolayer		

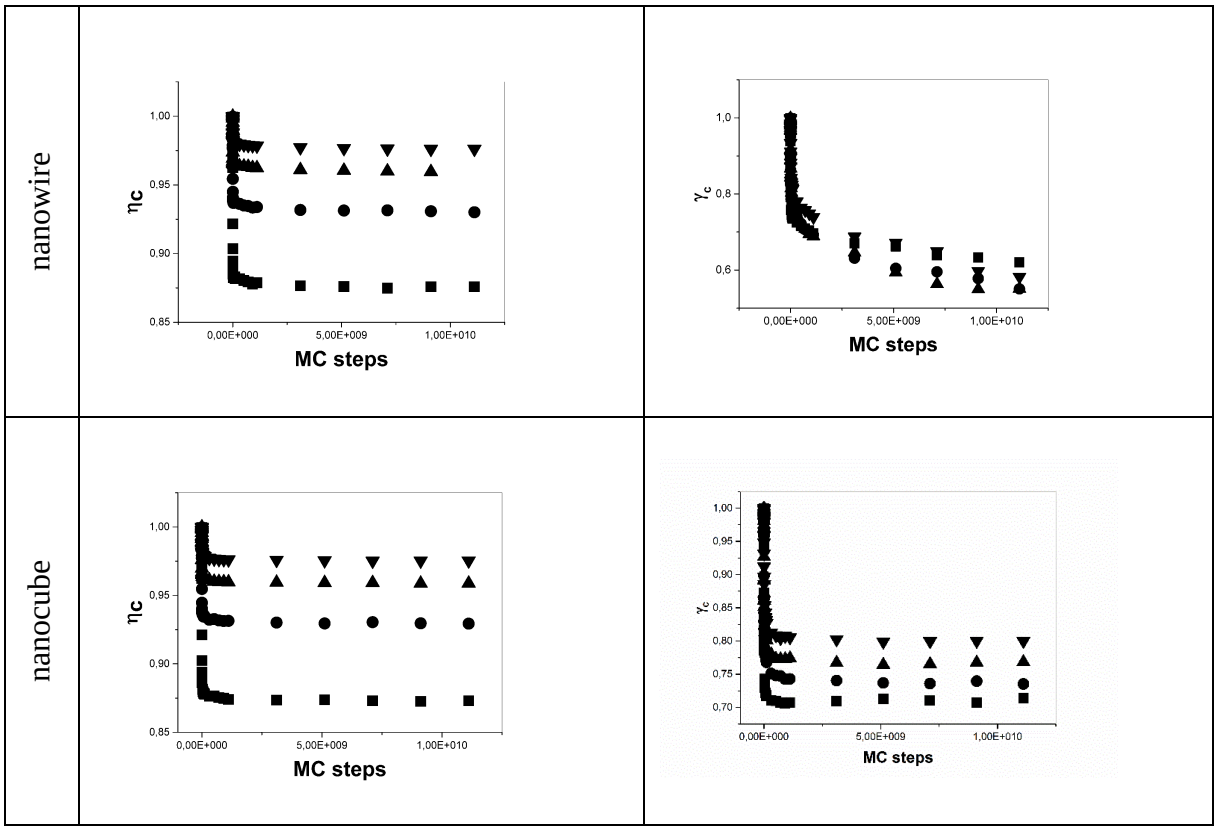


Figure 1 MC time-dependence of the LRO parameter η_c within the inner parts and of the c-$L1_0$ variant volume fraction γ_c in the PD-thick surface-affected parts of the samples at $T/T_T = 0{,}76$ (▼), $T/T_T = 0{,}83$ (▲), $T/T_T = 0{,}89$ (●) and $T/T_T = 0{,}95$ (■).

The graphs displayed in Figs. 2-4 show the temperature dependence of the volume fractions γ_x of the x-$L1_0$ variant domains in the nanolayer, nanowire and nanocube areas defined in the article in Table 4.

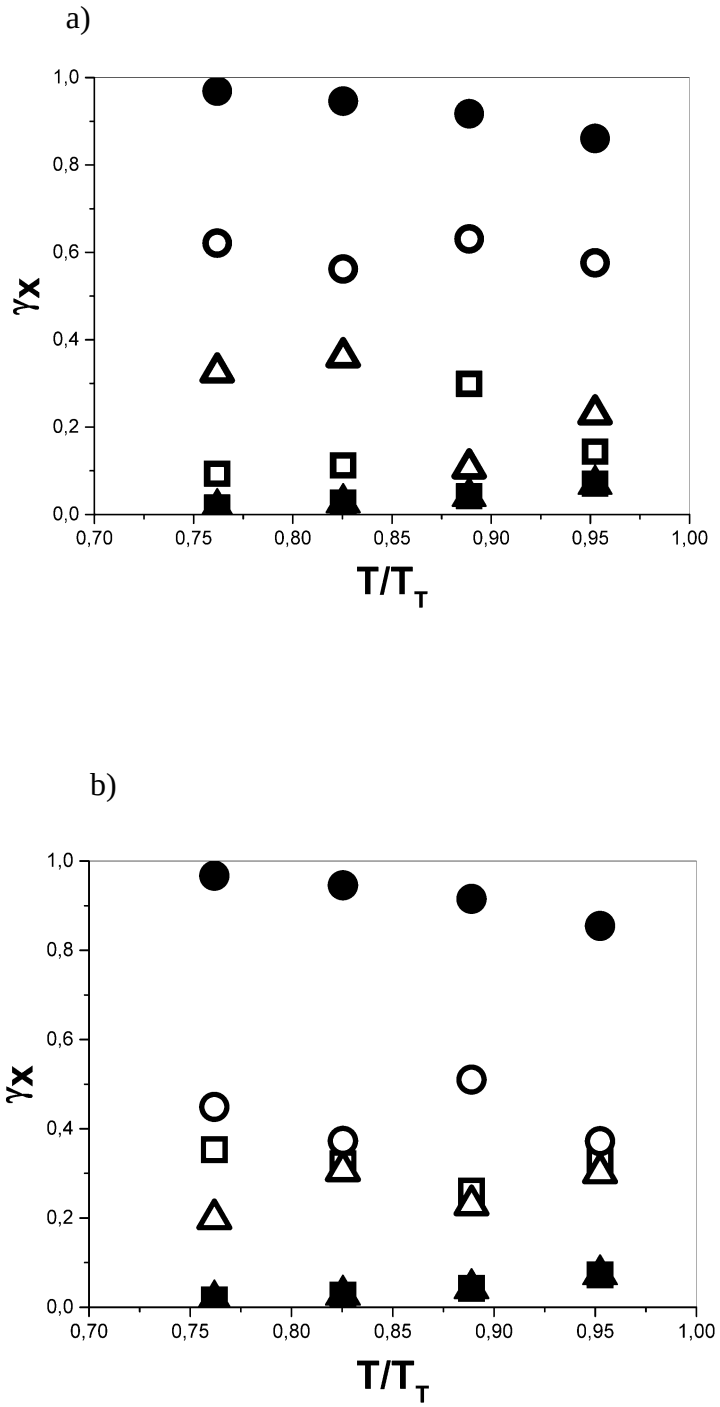
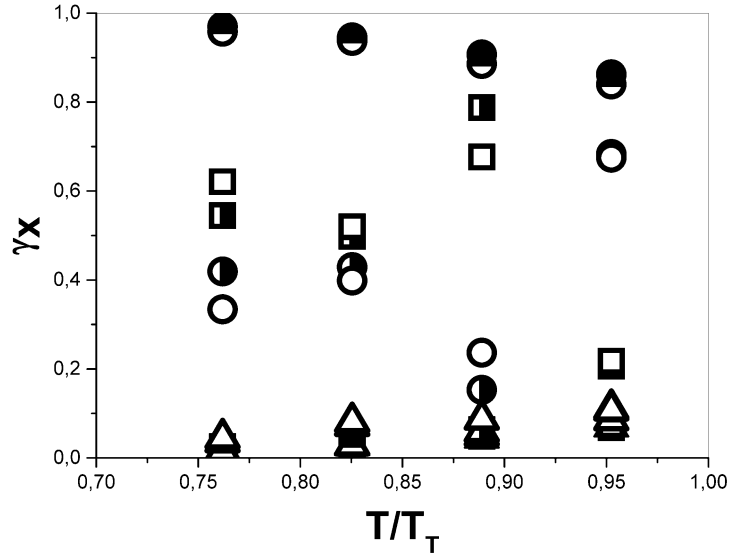


Figure 2 Temperature dependence of the $L1_0$-variant volume fractions γ_x in the nanolayer: (a) in a single sample; (b) averaged over 30 independent simulation runs. Solid and open symbols correspond to the inner part and the layer adjacent to the (001) surface, respectively. γ_a: (■,□); γ_b: (▲,△); γ_c: (●,○).

a)



b)

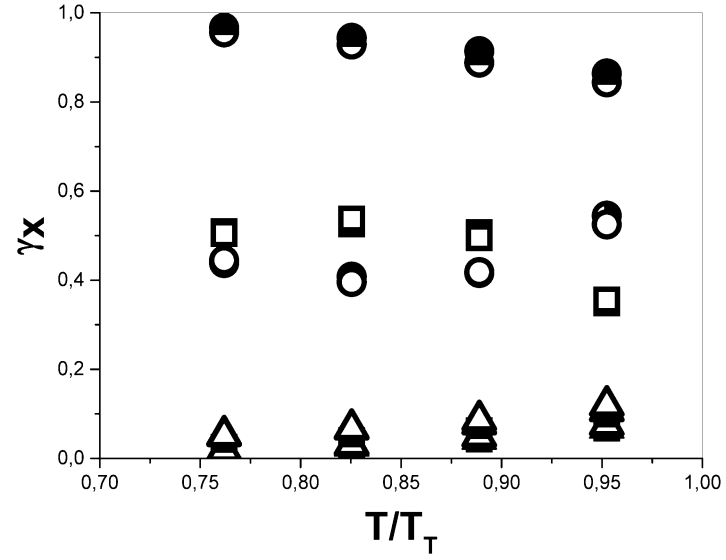
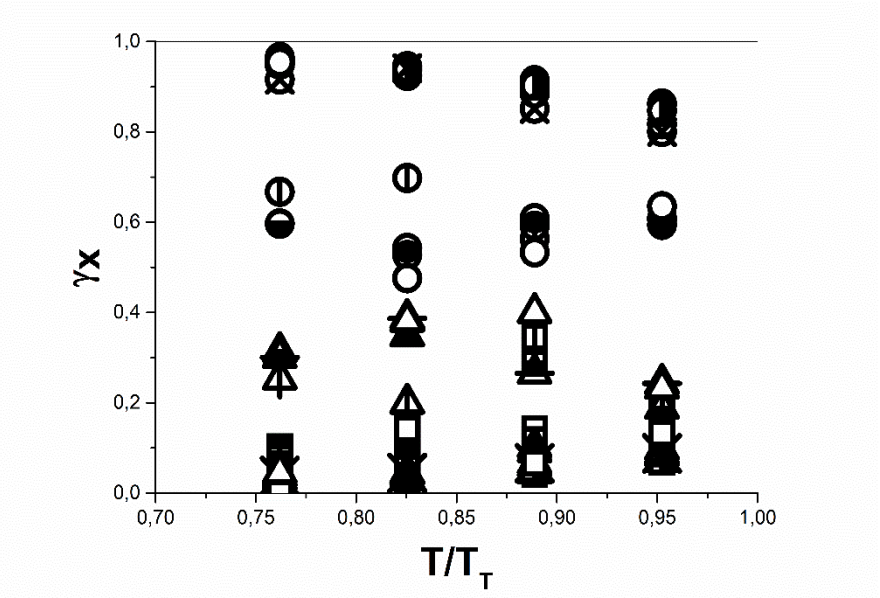


Figure 3 Temperature dependence of the $L1_0$-variant volume fractions γ_x in the nanowire: (a) in a single sample; (b) averaged over 30 independent simulation runs. Inner part: γ_a (■), γ_b (▲), γ_c (●); layer adjacent to the (010) surface: γ_a (⬒),γ_b (◬), γ_c (◓); layer adjacent to the (001) surface: γ_a (◨),γ_b (◭), γ_c (◑); [100] oriented edge area: γ_a (□), γ_b (△), γ_c (○).

a)



b)

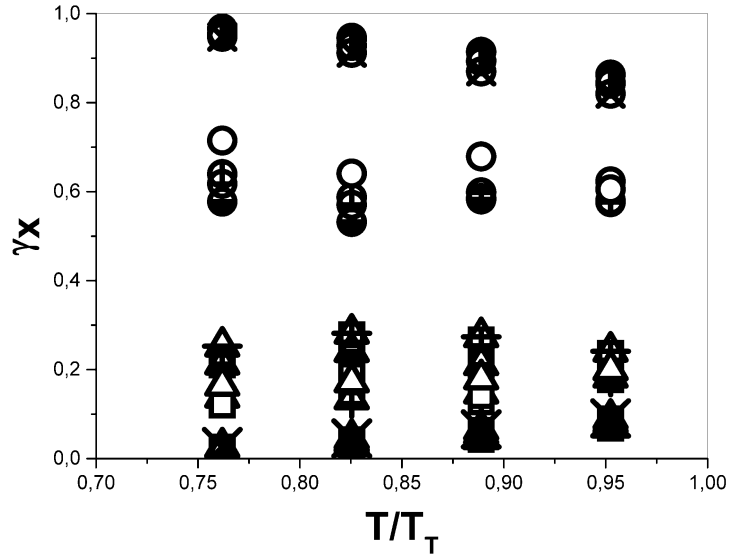


Figure 4 Temperature dependence of the $L1_0$-variant volume fractions γ_x in the nanocube: (a) in a single sample; (b) averaged over 30 independent simulation runs. Inner part: γ_a (■), γ_b (▲), γ_c (●); layer adjacent to the (100) surface: γ_a (⬒),γ_b (◬), γ_c (◓); layer adjacent to the (010) surface: γ_a (◨), γ_b (◭), γ_c (◑); layer adjacent to the (001) surface: γ_a (⬓), γ_b (◮), γ_c (◒); [100] oriented edge area: γ_a (◫), γ_b (⧋), γ_c (⓵); [010] oriented edge area: γ_a (⊟), γ_b (⧊), γ_c (⊖); [001] oriented edge area: γ_a (⊠), γ_b (⧓), γ_c (⊗); (111) vertex area: γ_a (□), γ_b (△), γ_c (○).