Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

The specific edge effects of 2D core/shell model for spin-crossover nanoparticles

AZUSA MURAOKA, Meiji University, KAMEL BOUKHEDDADEN, JORGE LINARÈS, FRANCOIS VARRET, Université de Versailles Saint-Quentin-en-Yvelines — We analyzed the size effect of spin-crossover nanoparticles at the edges of the 2D square lattices core/shell model, where the edge atoms are constrained to the high spin (HS) state. We performed MC simulations using the Ising-like Hamiltonian,

$$H = \sum_{(i,j)} S(i,j) S(i + i', j + j') + \left( \frac{\Delta}{2} - \frac{k_B T}{2 \ln g} \right) \sum_{(i,j)} S(i,j)$$

The molar entropy change is $\Delta S \approx 50J/K/mol$, $\ln g = \Delta S/R \approx 6$ (R is the perfect gas constant), energy gap is $\Delta = 1300K$. The HS fixed edges were based on the observation of an increasing residual HS fraction at low temperature upon particle size reduction. This specific boundary condition acts as a negative pressure which shifts downwards the equilibrium temperature. The interplay between the equilibrium temperature ($= \Delta / k_BT \ln g$) variation and the expected variation of the effective interactions in the system leads to a non-monotonous dependence of the hysteresis loop width upon the particle size. We described how the occurrence condition of the first-order transition has to be adapted to the nanoscale.

$^1$The present work has been supported by the Univ. Versailles, CNRS, GDRI France-Japan, and PRES-UniverSUd (COPECS project).

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Date submitted: 07 Dec 2011

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