



FIG. 1: (colors online) (a): body-centered tetragonal (BCT) lattice with  $J_0$  in-plane coupling constant, and out-of-plane  $J_1$ , and  $J_2$  competing interactions.

be achieved with different number of interacting layers: notably, nearest and next-nearest layers competitive interactions are enough to get a helical structure with a whatever pitch wavevector. Such observation gives us a possible way to solve the conundrum previously emerged, as we have the possibility of varying the range of interactions without modifying the helical pitch, thus decoupling the two relevant length scales along the film growth direction, and making accessible a range of  $n$  of the order of, or smaller than, the helical pitch, but still large enough that a substantial number of layers can behave as “bulk” layers. Therefore, while in the previous papers we have studied the properties of ultrathin magnetic films of Ho assuming a model with six interlayer exchange interactions, here we investigate by MC simulations the properties of the same system by making use of the simplest model Hamiltonian able to describe the onset of a helical magnetic order in Holmium, i.e. we consider only two inter-layer coupling constants, as previously done in Ref. 11.

The paper is organized as follows: In Sec. II the model Hamiltonian will be defined, and the MC techniques, and all the thermodynamic quantities relevant for this study, will be introduced. In Sec. III the results obtained for different thicknesses will be presented, both in the matter of the critical properties of the model and of the magnetic ordered structures observed. Finally, in Sec. IV we shall discuss such results, drawing also some conclusions.

## II. MODEL HAMILTONIAN AND MONTE CARLO OBSERVABLES

The model Hamiltonian we use in our simulations is the minimal one able to describe helimagnetic structures:

$$\mathcal{H} = - \left[ J_0 \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j + J_1 \sum_{\langle ik \rangle} \vec{S}_i \cdot \vec{S}_k + J_2 \sum_{\langle il \rangle} \vec{S}_i \cdot \vec{S}_l \right]. \quad (1)$$

$\vec{S}_i$  are classical planar unit vectors representing the direction of the total angular momentum of the magnetic ions, whose magnitude  $\sqrt{j(j+1)}$  ( $j = 8$  for Holmium ions) is already encompassed within the definition of the interaction constants  $J_{0,1,2}$ . As sketched in Fig. 1, the magnetic ions are located on the sites of a body-centered tetragonal (BCT) lattice; the first sum appearing in the Hamiltonian describes the in-plane ( $xy$ ) nearest neighbor (NN) interaction, which is taken ferromagnetic (FM), with exchange strength  $J_0 > 0$ ; the second sum represents the coupling, of exchange strength  $J_1$ , between spins belonging to nearest neighbor (NN) planes along the  $z$ -direction (which we will assume to coincide with the film growth direction); finally, the third sum takes into account the interaction, of exchange strength  $J_2$ , between spins lying on next-nearest neighbor (NNN) planes along  $z$ . In order to have frustration, giving rise to non-collinear order along  $z$  in the bulk, NN interaction  $J_1$  can be taken both ferro- or antiferromagnetic, but NNN coupling  $J_2$  has necessarily to be antiferromagnetic, and the condition  $|J_2| > |J_1|/4$  must be fulfilled. Such simplified Hamiltonian was already employed to simulate helical ordering in bulk systems by Diep<sup>1,17</sup> and Loison<sup>18</sup>. In the bulk limit, the state of minimal energy of a system described by Eq.(1) corresponds to a helical arrangement of spins. The ground state energy per spin is equal to  $e_g(Q_z) = [-4J_0 - 2J_1(4 \cos(Q_z c') + \delta \cos(2Q_z c'))]$  where  $c'$  is the distance between NN layers,  $\delta = \frac{J_2}{J_1}$ , and  $Q_z c' = \arccos(-\frac{1}{\delta})$  is the angle between spins lying on adjacent planes along the  $z$ -direction. The observed helical arrangement in bulk holmium corresponds to  $Q_z c' \simeq 30.5^\circ$ <sup>10</sup>: such value can be obtained from the formula above with the set of coupling constants  $J_0=67.2\text{K}$ ,  $J_1=20.9\text{K}$ , and  $J_2 = -24.2\text{K}$ , that we have employed in our simulations. The given values for the exchange constants are the same already used by Weschke *et al.* in Ref. 13 to interpret experimental data on Holmium films on the basis of a  $J_1 - J_2$  model, after a proper scaling by the numbers of NN and NNN on neighboring layers of a BCT lattice.

In the following we will denote with  $n$  the film thickness, i.e. the number of spin layers along the  $z$  direction, and with  $L \times L$  the number of spins in each layer (i.e.,  $L$  is the lattice size along both the  $x$  and  $y$  directions). In our simulations thickness values from 1 to 24 were considered, while the range of lateral size  $L$  was from 8 to 64. Periodic boundary conditions were applied along  $x$  and  $y$ , while free boundaries were obviously taken along the film growth direction  $z$ .

Thermal equilibrium was attained by the usual Metropolis algorithm<sup>19</sup>, supplemented by the over-relaxed technique<sup>20</sup> in order to speed-up the sampling of the spin configuration space: a typical “Monte Carlo step” was composed by four Metropolis and four-five over-relaxed moves per particle. Such judicious mix of moves is able both to get faster the thermal equilibrium and to minimize the correlation “time” between successive samples, i.e. the undesired effects due to lack of in-