METHODOLOGIES FOR NANO-GRAINS THIN FILMS SAMPLE CONSTRUCTION AND MONTE CARLO PARALLELIZATION FOR MAGNETIC ANALYSIS.

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One methodology for construction of thin films compound by nano-grains is presented. Size and shape of grains and sample are proposed under nano-scale considerations of magnetic materials. Periodic boundary conditions were taken into account. A comparative analysis with experimental grains distribution is presented. Lognormal distribution as function of number of atoms per grain is consistent with experimental reports. However distribution as function of grain diameter on the surface presents some differences mainly by the experimental measure processes at small diameters and limitations of grain size by sample dimensions. A test of the magnetization as function of temperature was obtained by Monte Carlo Parallelized through the subdivision of the sample. Hamiltonian considered variations of exchange constant with atomic distance from RKKY approximation, cubic magneto-crystalline anisotropy as function of the temperature and dipolar interaction with five replicas. The results show different values of magnetization of saturation at low temperature. These possible metastable states are independent of computational core numbers. Reduction of magnetization is correlated with mono-domain and multi-domain regimen in each grain and in the sample. The formation of these metastable states is mainly due to the combination of four essential factors: (i) the distance influence at short-range of exchange interaction, (ii) the existence of different favored magnetic moment directions caused by cubic anisotropy, (iii) the geometry and dimensions of the sample and finally (iv) the ratio between the number of atoms in the core vs. shell, according to the grain size and shape.

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