Computational Study of Magnetic Anisotropy Using Heisenberg Model and GPU-accelerated Monte-Carlo Simulation

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It has been difficult to predict complicate thermo-magnetic property of ferromagnetic materials using conventional DFT method due to its limitation to ignore thermo-magnetic spin fluctuation. This is because DFT originally doesn't have temperature variable in its Hamiltonian, and only considering zero-temperature electronic calculation. Thus, widely used ab-initio software based on zero-temperature Hamiltonian of DFT only takes experimental values of collinear magnetic moment measured in room temperature.

Alternative Monte-Carlo simulation based on Ising model has also been criticized due to its rough simplification of collinear spin direction, which makes it difficult to extend to large scaled atomic systems. First of all, Ising model is impossible to get the accurate physical pictures where spin is fluctuating with all orientation in spherical coordination rather than constrained with only up and down spin directions. Secondly, Monte-Carlo it self is very slow because it repeats random sampling for each iteration step which is critical issue to extend to the many atomic system.

Here, we developed new high-speed Monte-Carlo simulation package by implementing physically accurate Heisenberg model rather than Ising model. To accelerate the simulation, high performance feature using parallel distributed computing and Graphical Processing Units (GPU) has been implemented. The calculated figure of merit, Curie temperature shows good agreement with experimental values in test material tetragonal Fe system. Our GPU implementation runs 281 times faster (double precision; 749 times faster in single precision) than the sequential implementation on the Jinx nodes with the M2090 GPU cards for calculations of single Monte Carlo steps in 2D. In case of 3D stencil computation, It is shown that our GPU implementation runs 244 times faster than sequential algorithm. Both 2D and 3D stencil case, we have used checkerboard algorithm, which is interacting only with nearest neighboring threads in considering periodic boundary condition. The movement of spin has been optimized before the Monte-Carlo steps. We have implemented conventional Metropolis Monte-Carlo algorithm using Heisenberg model with optimized parameters.