Modelling magnetic walls in NiO

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NiO is a model antiferromagnetic of type G for its high transition temperature (T_N=523 K) and its simple rocksalt crystallographic structure. However, it has a complex magnetic structure, composed of T (favorite planes of spins) and S (favorite orientations of spin) domains. In the context of spintronic antiferromagnetic, the magnetic texture plays a key role. Magnetic transition zones such as T and S walls influence the overall behavior in spintronic devices. Understanding the transition zone between these structures are therefore critical.

Despite this criticity, a complete description at the atomic scale of the T and S wall is still missing. We fully simulate them, thanks to a Heisenberg Hamiltonian. We realized our simulations with Vampire, an atomic spin modelization software.

First, the superexchange constants were reassessed to obtain the experimental T_N. In order to obtain the type II antiferromagnetic structure, a linear relationship between atoms distance and first superexchange constants (J1) is implemented, coupled with a contraction along (111), used to simulate the magnetostriction and a set of two uniaxial anisotropy constant is used to describe S and T domain.

Second, we simulate 60°, 120° S walls and (100), (110) T walls by putting two domains side-to-side in the same simulation box.

A particular attention is given to the morphology of (100) T walls, created by the three different S domains from each side of the wall. From nine cases created by the variation of S walls from each side of the walls, three cases can be isolated. The general behavior of (100) T wall can be resumed in three steps for atomic spins.

1. A first in plane rotation from the departure direction to the shared direction between the two (111) plane of each domain T.
2. At the shared direction, the atomic spin split in two populations due to the antiferromagnetic structure of NiO.
3. These two population on goes a new in plane rotation in the other (111) plane to end at the arrival position.

The passage by the shared direction is the key to understand the magnetic behavior of NiO in magnetic transition zone. The behavior of (110) T walls are similar.

Some Nitrogen Vacancies Magnetometry (NVM) simulations were simulated for all walls.