Spin Orbit Coupling Effects on the Non-collinear Magnetism of Structurally Relaxed Fe/Cu (001) Thin Films: First Principles Calculations

R.Garibay-Alonso, J.L.Ricardo-Chávez, J.L.Rodríguez-López, and J.L.Morán-López

J. Mag. Mag. Mat., **514**, 167108 (2020)
https://doi.org/10.1016/j.jmmm.2020.167108

Highlights

- We present a study on the effects of the spin-orbit coupling interaction on the non-collinear magnetism of a Fe thin film of six monolayer thickness deposited on a Cu (001) substrate made of 12 atomic layers.
- Results reproduce the magnetic moment profile experimentally observed for the four Fe first layers in contrast with previous calculations.
- Also, an important aspect previously neglected, is that we included in our calculation structural relaxations, and found important changes in the intra-layer distances.

The effect of the spin–orbit coupling interaction and atomic relaxation, on the ground state non-collinear magnetism of deposited Fe thin films, on a Cu (001) surface, is studied by using first principles density functional theory calculations. The total energy values and spin and orbital magnetic local moments are calculated for a Fe film of N = 6 atomic layers deposited on a 12 layer thick Cu film playing the role of substrate. As a first step, we allow the thin film and surface layers to atomically relax. We found important contractions of about 20% between the first and second, the third and fourth, and firth and sixth Fe layers. Then, we obtain collinear and non-collinear magnetic arrangements which agree with the main experimental results state that show a non-collinear configuration at low temperatures (around 40 K). The magnetic properties of the first four Fe layers are well reproduced. The agreement is better than the results obtained ignoring the spin–orbit coupling and the structure relaxation. Although both calculations predict non-collinear configurations with energy values slightly above that of a collinear ground state. In some cases, the energy differences between two collinear (or non-collinear) solutions with different spin orientation axis is only under the value of one meV. The calculated orbital local moment arrangements are clearly similar to the spin magnetic local moment ones and show a correct dependence on the dimensionality aspects of the system when changing the spin axis quantization direction.