Lattice dynamics and magnetic structure of iron-based multilayers

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After the discovery of the antiferromagnetic (AF) exchange coupling between ferromagnetic (FM) layers separated by a nonmagnetic metal spacer, the interest in multilayer systems increased constantly over the last two decades. Among them, Fe/FeSi and Fe/Pt multilayer structures have become the subject of intense research in recent years.

These materials are very interesting from various points of view. The Fe/FeSi and Fe/Pt multilayers may provide new opportunities in material science and technology, if the orientation of magnetization in metallic Fe layers could be controlled by the actual multilayer composition. From a theoretical point of view the Fe based multilayers resemble critical phases in statistical mechanics.[1] However, the exact nature of the AF coupling between two metallic layers separated by a semiconducting/pseudometallic/insulating layer is still unclear.

In this work the magnetic properties of Fe/FeSi and Fe/Pt multilayers were investigated systematically by changing the thickness of Fe and FeSi layers in a periodic system consisting of four layers, i.e., two Fe and two FeSi (CsCl type) or Pt spacer layers interchanged with each other, with periodic boundary conditions. Several different starting configurations for the magnetization distribution were used in order to obtain unbiased results for a given system. In each case we determined the locally and globally stable configurations and next analyzed the results in order to extract information about the interlayer exchange couplings.

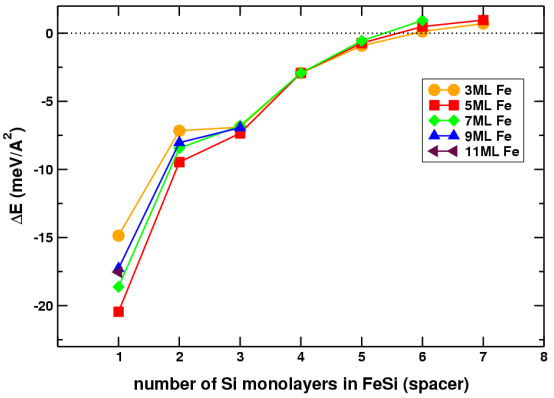

Fig 1: Difference of total system energy ΔE between the AF and FM configuration of the magnetic moments between two iron layers, separated by FeSi spacer of increasing size. Different data points for a fixed thickness of the spacer layer (number of Si monolayers) correspond to the systems with varying number of Fe ML (from 3 to 11) in each Fe layer.

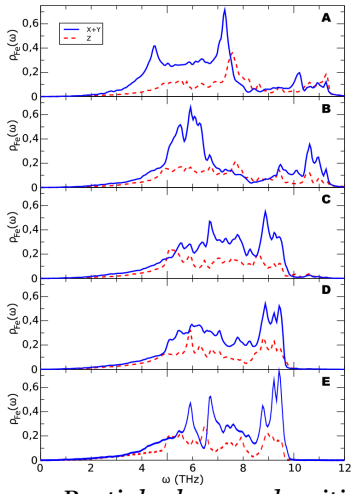

Fig 2: Partial phonon densities of states of the Fe/FeSi multilayer structure. Only iron atoms vibrations are included. The panels correspond to monolayers in the structure.

References

1. J. Pruneda, R. Robles, S. Bouarab, J. Ferrer, and A. Vega, Phys Rev B **65**, 024440 (2002).