AB INITIO STUDY OF INTERLAYER EXCHANGE COUPLING IN Fe/Si MULTILAYERS

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Interlayer exchange coupling has been studied from first principles in Fe/Si multilayers. The calculations have been performed in the framework of spin-polarized linear-muffin-tin method within supercell approach. Different structures with the spacer layer of thickness up to 15 atomic layers have been modeled from pure Si to $Fe_{50}Si_{50}$ alloy and including structures with isolated Fe impurities in the Si layer. Antiferromagnetic exchange coupling has been found for $Fe_{50}Si_{50}$ alloy spacer as well as for Fe-doped Si layer. The results of the modeling have been compared with the experimental data for Fe/Fe_xSi_{1-x} multilayers prepared by magnetron sputtering for x=1, 0.66 and 0.5. The dependence of antiferromagnetic exchange coupling on the spacer layer thickness up to 3 nm has been determined from the magnetization and Kerr effect measurements. The experimental results for the nominally pure Si spacer layer (x=1) can be explained assuming the Fe-doped Si model structure of the spacer layer. The magnetic moments and partial density of states for the model structures have been calculated and discussed.

9.7 cm

13.4 cm

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