Structure and magnetic anisotropy of  $Co \setminus Au(111)$  films

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Numerical calculations combined with the theoretical analysis, concerning  $Co \setminus Au(111)$ and  $Aq \setminus Co \setminus Au(111)$  thin films, aim at a microscopic interpretation of empirical data obtained by A. Maziewski and his group. The data show rather striking properties of surface and interface magnetism in these materials, and indicate their strong magnetic anisotropy. The structural and magnetic properties of thin Co films epitaxially grown on Au(111) substrates, are investigated using ab-initio local density calculations. It is shown that there is a large lattice intermismatch between Co and Au(111), which causes a growth mode of the polygonal Co islands of two atomic layers with a hcp structure. The lattice mismatch at the Co - Au interface leads to a buildup of the lattice strain. An enhancement of the magnetic moment on the free surface as well as at the  $hcp \ fcc$ interface is found. The influence of the capping Aq layers on the film's relaxation and on its magnetic moment has been also considered. In order to obtain energy of the magnetic anisotropy for the cobalt films, we perform relativistic spin-polarized local spin density calculations. We analyze an influence of Ag, which plays a prominent role as a substantial effect of the shape anisotropy in Co Au(111) films. It is also proved that magnetic anisotropy of Co/Au(111) and that of  $Ag \setminus Co \setminus Au(111)$  films essentially differ from each other.

— 13.4 cm –

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 $9.7 \mathrm{~cm}$