## EP08

# Magnetic Properties of Monolayer Co on W Substrates

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The 3d transition metals bcc Fe, hcp Co, and fcc Ni are known as the prototypical ferromagnets. Special attention has been given to magnetism of artificial crystalline ferromagnetic nanostructures. The artificial nanostructure is synthesized normally by growing a ferromagnetic overlayer on a paramagnetic substrate whose stable crystalline structure is different from that of the overlayer. Main factors to determine the magnetism of the artificial structure are its atomic structure and the strength of the hybridization with substrate [1]. Recently some interesting results were found. Fe films deposited on W(001) and W(110) substrates exhibit different magnetic ground states [2]. Their magnetic easy axis depends on the magnetic state; the easy axis of an antiferromagnetic (AFM) state is different from that of a ferromagnetic (FM) one. Magnetic mediation also depends on the substrate surface plane index.

In this study, we investigated the magnetism of monolayer (ML) Co on W(001) and W(110) substrates by means of the highly precise full-potential linearized augmented plane-wave (FLAPW) method, based on generalized gradient approximation (GGA). The Co atoms were calculated to be more stable on W(001) and W(110) in AFM and FM states by the energy differences of about 135 and 20 meV, compared to the corresponding FM and AFM ones, respectively. As shown in Fig. 1, the equilibrium Co-W interlayer distances in the FM and AFM states were calculated to be 3.707 and 3.599 a.u. [3.150 and 3.121 a.u.] for W(110) [W(001)]. (c.f. 3.41 a.u. in 1ML Co/W(110) in FM with FP-LMTO[1]). The detailed discussion on the origin of the different magnetisms will be given in the conference.

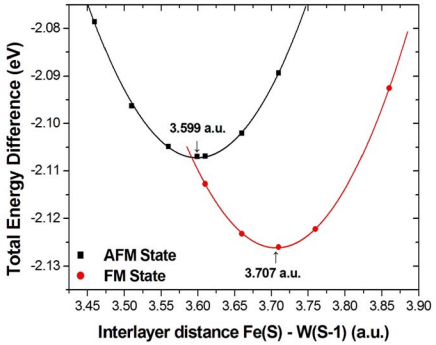


**Fig. 1.** Total energies of 1ML Co/W(110) in FM and AFM states as functions of the distance between the Co and the W surface.

**REFERENCES**

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## EP09

# Electronic Structures and Magnetic Properties of bcc Ni

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In stable fcc phase, Ni has a dominant magnetic character . However, in its metastable bcc phase, the magnetic character is greatly reduced indicating the possibility of superconductivity since superconductivity and magnetism are in general mutually completing properties. Recent progress in thin film growth techniques allows us to investigate metastable phases, which was hard to be synthesized before. In this presentation, we report magnetic and superconducting properties bcc Ni obtained by using the ab-initio band calculation. The results shows the possibility of stable nonmagnetic phase in bcc Ni under pressure. The stability of the nonmagnetic phase is also checked and compared with the case when other transition metal elements are doped to bcc Ni.

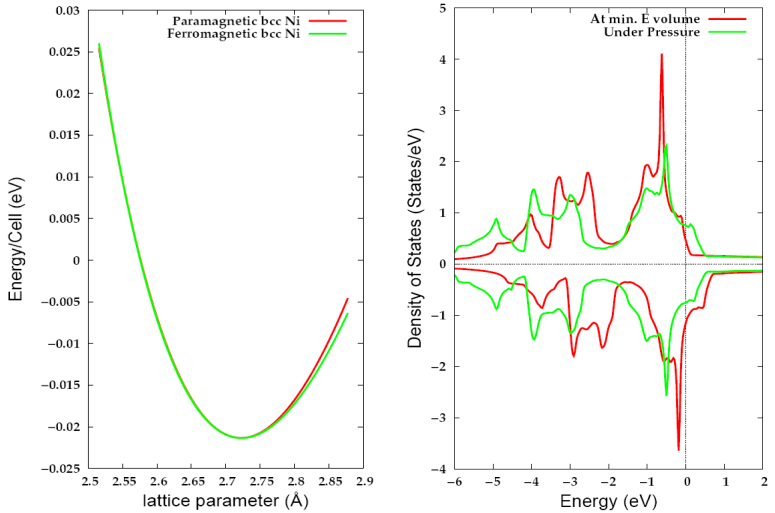


**Fig. 1.** (left) Energy vs lattice parameter graphs of bcc Ni in both paramagnetic and ferromagnetic phases (right) Density of states of minium energy volume and compressed volume.