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A study of magnetic overlayers of Fe on Cu(001)

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Abstract. Theoretical studies of the magnetic properties of Fe on Cu(001) as a function of coverage are reported.

Recent experiments on Fe epitaxial overlayers on Cu(001) have shown interesting structural and magnetic behaviour. For example, the Fe inter-layer spacing expands as the overlayer thickness increases [1], and the magnetisation drops [2]. To understand this, self-consistent surface electronic structure calculations have been carried out using the LMTO method applied to a supercell geometry and the embedded LAPW method applied to a semi-infinite system. Previous calculations have been carried out using the slab LAPW method [3]. The present calculations use lattice parameters [2] not previously theoretically modelled. The non-magnetic embedded LAPW calculations, applied to a

Table 1. Results of the LMTO calculations for an Fe monolayer (1 ML), bilayer (2 ML) and triple layer (3 ML) on Cu(001): non-magnetic layer-decomposed densities of states at the Fermi energy $N(E_F)$ (in states eV^{-1}/atom), layer-decomposed spin moment M_s (in μ_B/atom), averaged spin moment per Fe atom $\overline{M}_s$ (in μ_B) and magnetisation energy ΔE_M (in eV/Fe). Fe*n* and Cu denote the *n*th Fe overlayer and top Cu layer rspectively. Similar quantities for bulk Fe are also given for comparison.

	$N(E_F)$	M_s	$\overline{M}_s$	ΔE_M
1 ML	5.16 (Fe1)	2.73 (Fe1)	2.75	0.54
	0.46 (Cu)	0.02 (Cu)		
2 ML	2.54 (Fe2)	2.68 (Fe2)	2.49	0.25
	2.63 (Fe1)	2.30 (Fe1)		
	0.33 (Cu)	0.03 (Cu)		
3 ML	3.71 (Fe3)	2.70 (Fe3)	2.29	0.22
	2.14 (Fe2)	1.86 (Fe2)		
	3.19 (Fe1)	2.30 (Fe1)		
	0.53 (Cu)	0.03 (Cu)		
Bulk Fe	3.65 (BCC)	2.20		0.43
	2.15 (FCC)	0.0		

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monolayer of Fe, give a large work function of 5.75 eV, in good agreement with the experimental value of 5.5 eV. The density of states on the Fe overlayer has a big peak at the Fermi energy, clearly indicating the possibility of a ferromagnetic instability, and the substrate Cu d band is considerably distorted from the bulk. This is confirmed by the LMTO calculation using five Cu layers sandwiched between two Fe layers plus five vacancy layers.

When spin polarisation is allowed in the LMTO calculation, a monolayer of Fe on the Cu(001) shows a moment of 2.73 μ_B/Fe in agreement with the full potential LAPW method (2.85 μ_B) [3]. Moreover the density of states is almost identical with that from the LAPW calculations—this is very encouraging as the LMTO method, which uses spherically averaged potentials, is by far the most economical method available. We were therefore able to study the magnetic properties as a function of overlayer thickness obtaining the results summarised in table 1. These results show that the averaged magnetic moment drops with increasing Fe coverage, presumably because the centre of the overlayer resembles FCC Fe which is non-magnetic. The trend is in agreement with the experiment [2] although the calculated values are systematically too large by about 0.4 μ_B/Fe.

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