ESRF	**Experiment title: Atomic Structure in Magnetic Nanocomposite Co/Mn Films.**	**Experiment number**: HE-2642
Beamline: BM29	**Date of experiment**: from: 07/02/2008 to: 10/02/2008	**Date of report**: 03/07/2008
Shifts: 9	**Local contact(s)**: Dr Sakura Pascarelli	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Dr S.H.Baker* University of Leicester, UK.
Dr M.Roy* University of Leicester, UK.
Mr S.Rhead* University of Leicester, UK.
Prof. C.Binns University of Leicester, UK.

Background and Experimental

The potentially high moments in magnetic cluster-assembled materials offer much promise for new high performance magnetic materials. However, the low blocking temperatures in magnetic nanosized clusters is clearly a problem. One approach to solving this is to embed the clusters in an antiferromagnetic (AF) material (with a sufficiently high Néel temperature - T_N). Recent magnetic susceptibility measurements by us on films of Co clusters embedded in Mn [1] show that the blocking temperature in the Co clusters is 65K – an appreciable increase on ~10K that we measured for Co clusters in non-magnetic Ag. This indicates that the AF Mn matrix (for which T_N = 95K) provides strong interface exchange coupling with the ferromagnetic Co clusters. However, for magnetic clusters embedded in a matrix, the choice of matrix material can affect the crystal structure of the clusters, and hence play a critically important role in determining their magnetic properties. For example, using EXAFS and magnetometry, we have shown that at low filling fractions (VF) (i) Co clusters in Fe switch to a higher moment bcc structure (c.f. hcp in bulk Co) [2] (ii) Fe clusters in Cu adopt a low spin fcc structure (c.f. bcc in bulk Fe) [3]. Here we report on EXAFS experiments performed to investigate the atomic structure of Co clusters embedded in Mn. The embedded cluster films were prepared by co-depostion using a UHV-compatible gas aggregation cluster source, on Si(100) substrates. Co and Mn K edge EXAFS measurements were performed in fluorescence on BM29. During data-collection, a rotating sample holder was used which ensured that diffraction "spikes" from the substrate were absent from the measured spectra. The data were analysed using the EXCURV98 program.

Co K Edge Results

Fig.1 shows the Co K edge EXAFS χ, weighted by k^3, and associated Fourier Transform for a film containing 11.5% VF of Co clusters in a Mn matrix. The same information for a Co MBE film is shown in fig.2. The first point to note is the much reduced amplitude of the EXAFS in the embedded cluster film compared with that measured for the Co MBE film. This suggests appreciable alloying between Co and Mn. An outer shell of CoMn alloy, with some structural disorder i.e. variation in interatomic distances, surrounding a reduced Co core would produce a spread of nearest neighbour distances; interference between overlapping contributions will reduce the amplitude of the measured EXAFS. [A good hcp fit was obtained to the Co MBE film data].

CoMn alloys, both AF with an fcc structure and also ferromagnetic with a bcc structure can be grown epitaxially on GaAs(001) [4]. Our magnetic data [1] show that the average atomic moment per atom in the embedded Co clusters is much reduced relative to bulk Co, indicating that the CoMn shell is AF and that only a small fraction of the Co atoms at the core remain unalloyed. The EXAFS analysis is of course

hampered by the fact that Co and Mn atoms scatter similarly. However, the fit to the data in fig.1 is consistent with two contributions: (1) 8.7 ± 2.9 atoms at a distance r_1 = 2.55 ± 0.04 Å with a Debye-Waller factor $2\sigma_1^2$ = 0.048 ± 0.016 Å^2 (2) 0.6 ± 0.9 atom at a distance r_2 = 2.39 ± 0.03 Å with a Debye_waller factor $2\sigma_2^2$ = 0.002 ± 0.016 Å^2. The contribition at 2.55 ± 0.04 Å implies an fcc lattice parameter of 3.61 ± 0.06 Å, consistent with values reported elsewhere [5] for AF fcc CoMn alloys. The nearest neighbour distance in the pure unalloyed Co core will be 2.50–2.51 Å if the structure remains hcp; if so, this will be included in the main fit contribution. The second fit contribution at 2.39 ± 0.03 Å is much shorter than this, although a little closer to 2.45 ± 0.01 Å measured for bcc Co clusters [3]. However, it is worth noting that the α–Mn structure has nearest neighbour contributions at 2.35 Å and 2.42 Å (among others) [5]; at the outer edge of the CoMn alloy shell, the crystal structure could resemble the α-Mn one. Data and fit results for a 41.3% VF Co/Mn film, where VF > ~ 25% - the 3-D percolation threshold, are similar to those shown for the 11.5% VF film; this indicates that alloying is appreciable in larger agglomerates of Co clusters as well as in isolated clusters.

Mn K Edge Results

Figs.3 and 4 show Mn K edge EXAFS data for a 5.0% VF Co/Mn film, and for a Mn MBE film respectively. Again, we notice the reduced amplitude of the EXAFS compared to that for the Co MBE film; this indicates that there is a significant number of overlapping shells. The data in figs.3 and 4 resembles that published elsewhere for α-Mn [6], which has a complex structure containing 58 atoms in the unit cell and with 4 different i.e. non-equivalent sites for the absorbing atom. The maximum number of statistically significant shells that we were able to fit to the Mn edge data was three, with contributions at 2.38 ± 0.03 Å 2.68 ± 0.02 Å and 4.21 ± 0.03 Å for the 5.0% VF Co/Mn film, and 2.40 ± 0.02 Å, 2.70 ± 0.02 Å and 4.25 ± 0.05 Å for the Mn MBE film. These are consistent with known interatomic distances in the α-Mn structure [5].

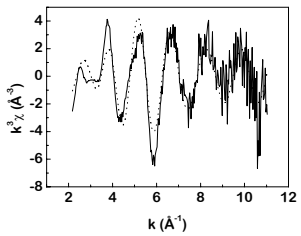
Summary

Co clusters embedded in a Mn matrix are subject to alloying. By combining the results of EXAFS and magnetic experiments, we deduce that an AF fcc CoMn alloy outer shell surrounds a much reduced pure Co core. The matrix has the α-Mn structure. The EXAFS results will shortly be submitted for publication in combination with results of spin-polarised electronic structure calculations on the Co/Mn system.

References

[1] N.Domingo, A.M.Testa, D.Fiorani, C.Binns, S.Baker, J.Tejada (2007) J.Magn.Magn.Mater.**316** 155
[2] S.H.Baker, M.Roy, S.Louch, C.Binns, (2006) J.Phys.:Condens.Matter **18** 2385
[3] S.H.Baker, A.M.Asaduzzaman, M.Roy, S.J.Gurman, C.Binns, J.A.Blackman, Y.Xie (2008) Phys.Rev.B
[4] D.Wu, G.L.Liu, C.Jing, Y.Z.Wu, D.Loison, G.S.Domg, X.F.Jin (2001) Phys.Rev.B **63** 214403
[5] J.A.Oberteuffer and J.A.Ibers (1970) Acta Crystallographica B **26** 1499
[6] S.Andrieu, H.M.Fischer, M.Piecuch, A.Traverse, J.Mimault (1996) Phys. Rev.B **54** 2822

Figures [In all figures: Full line – data. Dotted line – fit]



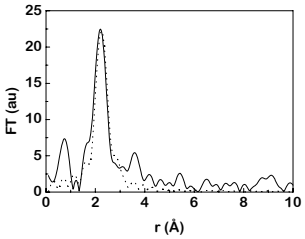
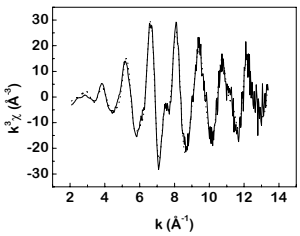


Fig.1 Co K edge EXAFS data for 11.5% VF Co/Mn Film



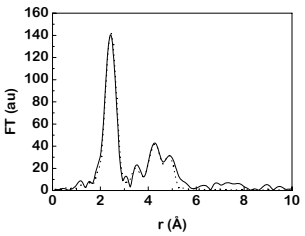
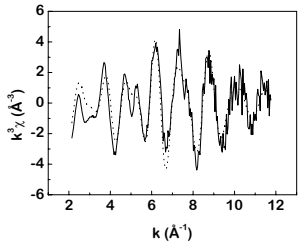


Fig.2 EXAFS data for Co MBE Film



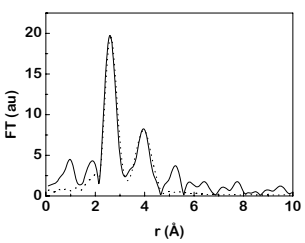
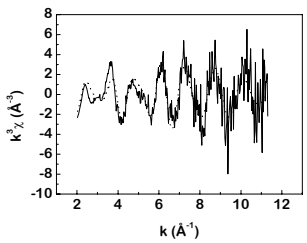


Fig.3 Mn K edge EXAFS data for 5.0% VF Co/Mn Film



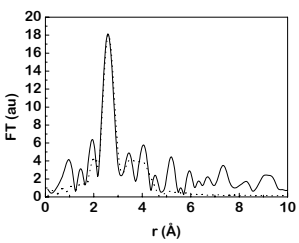


Fig.4 EXAFS data for Mn MBE Film