FA2-MS06-O1

Shape Reconstruction of Nanoparticles under Reaction Conditions. Andreas Stierle. *Max-Planck-Institut für Metallforschung, Stuttgart, Germany.*
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Substantial effort has been made within the past few decades to understand the fundamentals of oxidation using pioneering-type experiments under highly idealized conditions, such as very low oxygen pressures (10^{-6} mbar), and very idealized model systems (single crystal surfaces). However, understanding chemical reactions on single crystal surfaces in vacuum very often does not allow prediction of the performance of devices composed of nanoparticles operating at ambient gas pressure, such as catalysts or gas sensors. In my talk I will present a systematic investigation of model systems with increasing complexity (single crystal & vicinal surfaces, epitaxial nanoparticles on single crystal oxide supports). I will demonstrate how synchrotron radiation based x-ray diffraction can be performed under near-atmospheric pressures and elevated temperatures, providing atomistic inside into the structure of metal nanoparticles during oxidation and reduction cycles. Recent results on the shape reconstruction of Rh nanoparticles on MgO(100) will be discussed [1].

[1] Nolte P., Stierle A., Jin-Phillip N. Y., Kasper N., Schulli T. U., Dosch H., *Science* 321, **2008** 1654.

Keywords: nanoparticles; synchrotron radiation; chemical reactions

FA2-MS06-O2

The Influence of Interfaces on the Properties of Magnetic Nanoelements and Wires. John Chapman. *Department of Physics and Astronomy, University of Glasgow, Glasgow, UK.*
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Magnetic nanoelements and wires are used widely in sensing and storage devices [1]. To obtain the necessary performance as critical dimensions of nanoelements enter the 100 nm regime, it becomes necessary to use multilayer films and to pay ever increasing attention to the physical microstructure and the nature of interfaces. Moreover the fabrication method used to form the nanoelements becomes a matter of concern as damage at the surfaces can lead to magnetic instability or a reduction in transport properties. Here I describe how the magnetisation processes in magnetic nanoelements are influenced by the underlying microstructure. Electron imaging reveals both the magnetisation distribution in the film (resolution of the order of 10 nm) and the local structure and composition (resolution of the order of 0.2 nm). Moreover in situ experimentation involving changing magnetic fields or spin-polarised currents can be readily undertaken. By way of example I consider the propagation of head-to-head domain walls (DWs) down magnetic wires fabricated from a soft magnetic film. Variable behaviour in nominally identical wires can be attributable to stochastic processes of thermal origin and inevitable variations in grain structure. I describe how the origin of the non-reproducibility can be probed and suggest ways of minimising its effect. The structure of the DW itself is important and it is possible to observe directly vortex and transverse DWs each of which can exist in a number of degenerate forms. Whilst such degeneracy is unimportant in regular lengths of straight wire, it becomes crucial when domain wall traps, an integral part of many devices, are present. Micromagnetic modelling complements the direct TEM observation by providing insight into how processes too fast to observe take place.

[1] Parkin S.S.P., Hayashi M., Thomas L., *Science,* **2008**, 320, 190.

Keywords: magnetic nanoelement; TEM; domain wall

FA2-MS06-O3

The Structure and Magnetism of Fe/Mo(001) Surface: A Pseudopotential Calculation. Amall Ahmed Ramanathan[a], Jamil M. Khalifeh[a], Bothina A. Hamad[a]. [a]*Department of Physics, University of Jordan*, *Amman.*
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The effect of structure on the magnetism of iron (Fe) monolayer (ML) on Molybdenum (Mo) is investigated using the Density Functional Theory (DFT) with norm conserving pseudopotentials (NCPP's) and a plane wave basis, under the Local Spin Density Approximation (LSDA). Relaxation of 5 ML and 7 ML of Mo resulted in a contraction of 11.3% and 11.7%, respectively, for the top Mo-Mo interlayer spacing in close agreement with experimental results. In the case of one Fe overlayer, the top Fe-Mo interlayer spacing contracted by 15.8% for a FM p(1x1) and 20.6% for a AF c(2x2) configuration. The magnetic moment of the surface (Fe) layer is enhanced from its theoretically calculated bulk value. Total energy calculations show the AF c (2x2) to be the stable state with a magnetic moment of $2.53\mu_B$. The surface Fe atoms are anti-ferromagnetically (AF) coupled with each other and with the Mo layers, showing layered AF. The present study demonstrates the reliability of pseudopotential approach under LSDA with core corrections included to the calculation of magnetic properties of combined transition metal systems.

Table1. Percentage interlayer spacing Δij for 7 layers

Fe/Mo(001)	This work	FLAPW[c]
$\Delta 12$	-15.8[a]; -20.6[b]	-13.9
$\Delta 23$	-0.04[a]; 1.97[b]	
$\Delta 34$	0.90[a]; 0.57[b]	

Table2. Magnetic moments in units of (μB) in the different layers.

	S	S-1	S-2	C
This work Fe/Mo(001)[a] Fe/Mo(001)[b]	2.79 2.53	-0.25	0.16	-0.18
Fe/W(001)[c]	2.67			