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			

[a] FM p(1×1)calculations
[b] AF c(2×2) calculations
[c] Tunneling Microscopy and FLAPW [Ref.1]

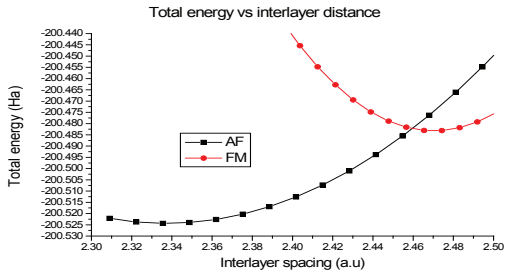

Fig.1

[1] A. Kubetzka, P. Ferriani, M. Bode, S. Heinze, K. von Bergmann, O. Pietzsch, and R. Wiesendanger[1] S. Blügel and G. Bihlmayer, *Phys. Rev. Lett.* 94, 087204, **2005**.

Keywords: magnetism; DFT; pseudopotential

FA2-MS06-O4

GISAXS-based Optimization of La/B_4C Multilayer Mirrors for Soft X–ray FEL. Matej Jergel[a], Peter Siffalovic[a], Eva Majkova[a], Livia Chitu[a], Stefan Luby[a], Karol Vegso[b], Stefan Hendel[c], Maike Lass[c], Marco D. Sacher[c], Wiebke Hachmann[c], Ulrich Heinzmann[c], Andreas Timmann[d], S. V. Roth[d]. [a]*Institute of Physics SAS, Bratislava, Slovak Republic.* [b]*Faculty of Mathematics, Physics and Informatics, Comenius University, Bratislava, Slovak Republic.* [c]*Faculty of Physics, University of Bielefeld, Bielefeld, Germany.* [d]*HASYLAB/DESY, Hamburg, Germany.*
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Lanthanum based multilayer mirrors are a convenient choice for the soft X-ray energy range. In additon to conventional periodic mirrors, aperiodic (chirped) broadband multilayers are needed to process extremely short light pulses from free-electron lasers (FELs) or high harmonic laser radiation. Here, smooth and narrow interfaces are of primary importance.
Ion beam polishing (IBP) proved to be an efficient way to enhance the interface quality in multilayers. UHV electron beam evaporation is one of the few techniques compatible with IBP. We studied the effect of IBP with Kr^+ ions in UHV deposited La/B_4C multilayers. These multilayers are applicable in the 100-190 eV energy range which fits well the spectrum of FLASH facility in Hamburg. Periodic multilayers (nominal period 3.5 nm) were chosen for pilot studies to facilitate evaluations.
Basic multilayer parameters were obtained from the specular X-ray reflectivity completed by high-resolution transmission electron microscopy. Grazing incidence SAXS (GISAXS) measurements were performed at HASYLAB BW4 beamline. Analyses of GISAXS patterns (Fig. 1) showed presence of vertically correlated and uncorrelated roughness with lateral periods of ~42 nm and ~13 nm, respectively. The ability to reveal coexistence of both types of roughness is a unique feature of GISAXS. The polishing of La layers brought about a reduction of both lateral and vertical roughness correlations starting from high frequencies and suppression of the diffuse scattering while the polishing of B_4C layers had negligible effect. The implications for preparation of chirped La/B_4C multilayers are straightforward.

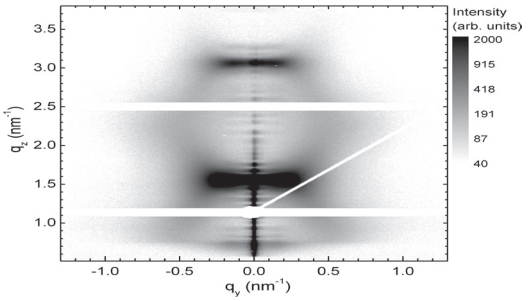

Fig. 1 GISAXS pattern of an unpolished sample. White stripes are "stitches" of the Pilatus 300K detector. (λ = 0.138 nm, $\alpha_{incidence}$ = 0.7 degree)

Keywords: FEL free electron lasers; GISAXS; multilayer structures

FA2-MS06-O5

Structure of the Surface Oxides Grown on the Icosahedral Al-Pd-Mn Quasicrystal. Mehmet Erbudak[a,b], Sven Burkardt[b]. [a]*Department of Physics, Boğaziçi University, Istanbul.* [b]*Lab. Solid State Physics, ETHZ, CH-8093 Zurich.*
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Determination of the crystal structure of oxides grown on ordered aluminum binary alloys have been an immense challenge for scientists since decades. It was found that oxygen binds to Al and forms an atomically thin Al-oxide layer in a corundum-related structure, modulated by contributions from an unusually large surface reconstruction and antiphase domain boundaries [1,2].
Here we report the structure of crystalline oxide layers grown at elevated temperatures on the pentagonal surface of the icosahedral Al-Pd-Mn quasicrystal. We have used Auger electron spectroscopy for chemical information about the surface layers. The results show that only Al binds to O, while Pd and Mn remain unaffected by O. Surface-sensitive structural information is extracted from patterns of low-energy electron diffraction, LEED. Owing to the lack of periodic order in quasicrystals, there is a strong structural mismatch at the quasicrystal-oxide interface which results in strong strain fields in atomically thin pseudomorphic layers. For thicker layers, the strain is relaxed by decomposing the film into 3 – 4 nm large domains. LEED patterns further confirm the formation of five distinct azimuthal orientations of domains indicating that the domains are locked to the fivefold-symmetric structure of the substrate. The major signal from each domain confirms the presence of a sixfold-symmetric atomic order as expected from the (111) surface of the hexagonal structure, which is characteristic to most of the corrundum