^a FM p(1×1)calculations

^bAF c(2×2) calculations

^cTunneling Microscopy and FLAPW [Ref.1]

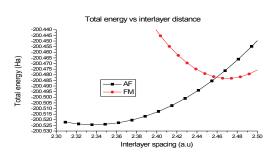


Fig.1

[1] A. Kubetzka, P. Ferriani, M. Bode, S. Heinze, K. von Bergmann, O. Pietzsch, and R. Wiesendanger¹ S. Blügel and G. Bihlmayer, *Phys. Rev. Lett.* 94, 087204, **2005**.

Keywords: magnetism; DFT; pseudopotential

FA2-MS06-O4

GISAXS-based Optimization of La/B₄C 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. *Institute of Physics SAS, Bratislava, Slovak Republic. *Faculty of Mathematics, Physics and Informatics, Comenius University, Bratislava, Slovak Republic. *Faculty of Physics, University of Bielefeld, Bielefeld, Germany. *dHASYLAB/DESY, Hamburg, Germany.

E-mail: jergel@savba.sk

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 $_4\mathrm{C}$ 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 B₄C layers had negligible effect. The implications for preparation of chirped La/B₄C multilayers are straightforward.

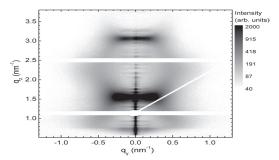


Fig. 1 GISAXS pattern of an unpolished sample. White stripes are "stitches" of the Pilatus 300K detector. (λ = 0.138 nm, $\alpha_{incidence}$ = 0.7 degree)

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. ^aDepartment of Physics, Boğaziçi University, Istanbul. ^bLab. Solid State Physics, ETHZ, CH-8093 Zurich.

E-mail: erbudak@phys.ethz.ch

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 Aloxide 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

phases. We observe additionally, that moderate oxidation makes the surface oxide layer reconstruct in the form of $2\sqrt{3}$ (1x1) – R30° which produces a unit cell that is 12 times larger than that of the unreconstructed hexagonal corundum structure. As the oxidation procedes, the diffraction patterns are strongly modulated by the contribution of antiphase boundaries separating the domains. It is essential to keep the temperature around 700 K while oxidation in order to promote Al segregation to the surface that required for the formation of the oxide. We make attemps to understand these observations in terms of structural details of the quasicrystal-oxide interface. We also emphasize the possibility of using these well-ordered islands as substrates for generating quantum-wells [3]. Since the film thickness can easily be controlled, these interfaces help us investigate finite-size effects in quantum-well structures.

[1] Kresse G. et al., *Science* **2005**, 308, 1440. [2] Stierle A. et al., *Science* **2004**, 303, 1652. [3] Burkardt S., Erbudak M., Maeder R., *Surf. Sci.* **2009**, 603, 866.

Keywords: oxide surfaces; low-energy electron diffraction; quasicrystals