PS-11.01.16 X-RAY REFLECTIVITY CHARACTERIZATION OF SURFACES, INTERFACES AND MULTILAYERS.

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Characterization of surfaces, interfaces and thin films is a growing and important application of X-ray analysis. X-ray results can be used to develop methods of growth of materials and in the interpretation of their physical properties.

In our laboratories, the X-ray reflectivity technique has been used successfully for the characterization of surface smoothness and oxidation, interface roughness and diffusion, layer thickness and density of sputtered polycrystalline and molecular-beam epitaxial films. Specular reflectivity data from below to several degrees above the critical angle for total reflection were collected using Cu X-rays and analyzed by least squares refinement. Results are summarized as follows:

SURFACES: Thin layers of native oxides were found on metal surfaces. The thicknesses of the oxides varied from about 20 angstroms and more for Ni, Si and Ta to 10 angstroms and less for Pt. Comparing to their thicknesses, the surface roughnesses were small for thick Ni, Si and Ta oxides. The roughness/thickness ratios for these oxide surfaces were about 30% and less. The roughnes/thickness ratios for Pt oxides were, however, much higher at about 50% and more. The observed large roughness/thickness ratios for thin Pt oxides suggested nonuniform oxidation on the surfaces of the noble metal.

INTERFACES: The roughnesses (or widths) of buried interfaces were found to be 25 angstroms and less depending on materials and preparation conditions. The widths of most buried interfaces were found to increase with annealing temperatures, indicating significant expansion of interfacial mixing at layer boundaries caused by interdiffusion. For example, the interfacial widths between Cu and NiFe in a giant-magnetoresistance multilayer of Ta/FeMn/NiFe/Cu/NiFe/Ta deposited on a Si substrate increased more than three times from 7 to 24 angstroms after annealing at 360C for six hours. The increase in widths was correlated with the increase in thicknesses in the magnetically inactive layers detected previously in NiFe.

LAYERS: Layer thicknesses were determined with high precise, and the standard deviations were estimated to be in the 0.1-angstrom range. The densities of most buried layers were found within 10% of the bulk densities. Unusual layer densities for Co in epitaxial films composed of alternate layers of very thin Co (2-5 angstroms) and much thicker Pt (18 angstroms) were also observed. The densities were more than 30% higher than that of the Co bulk density, suggesting a mixture of heavy Pt atoms in Co. Similar mixing of Pt in Co was also observed by angle-resolved X-ray photoelectron spectroscopy.

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PS-11.01.17 LATTICE-ADAPTABLE SUBSTRATES FOR $YBa_2Cu_3O_x$

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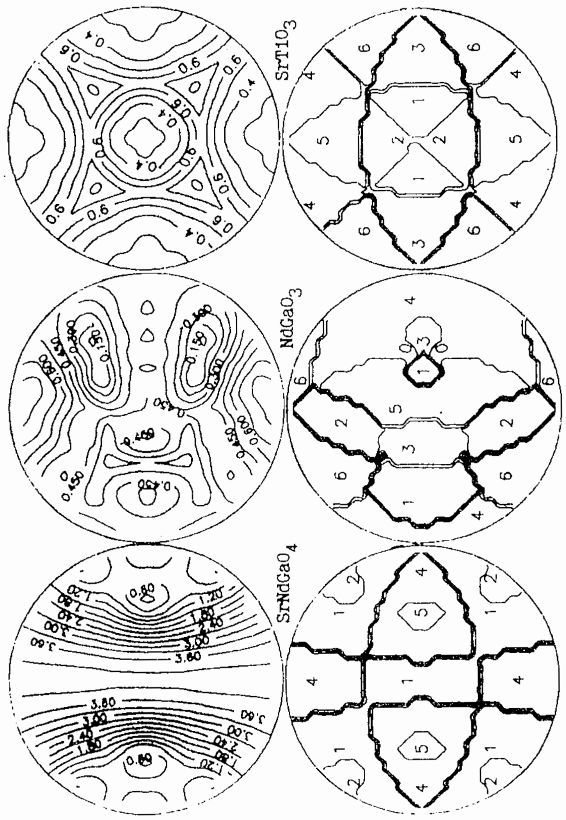
Both lattice mismatch and stereographic maps of epitaxial relationships "HTS on perovskite-type substrates" have been considered as a function of substrate orientation for $SrTiO_3$ and families $Ln(Al,Ga)O_3$ and $(Ca,Sr)Ln(Al,Ga)O_4$, where Ln- rare-earth element. The compositions and orientations of substrates needed to create perfect HTS-layers are presented.

Table 1. Planes of minimum misfit for the perovskite-type substrates

Phase		Minimum misfit plane	Misfit,%
$SrTiO_3$	a=3.898	(100)	0.33
$LaAlO_3$	a=3.792 α=90.067	(37.8; 0.76; 2.3)	1.66
$SrLaAlO_4$	a=b=3.75 c= 4.167	(1; 0; 1.297)	1.26
$NdGaO_3$	a=c=3.864 b=3.855 β=90.713	(15.9; 22.4; 26.9)	0.03
$LaGaO_3$	a=c=3.8982 b=3.8778 β=90.569	(1.557; 0; -1)	0.01
$SrLaGaO_4$	a=b=3.847 c=4.227	(1; 0; 3.768)	0.32
$CaNdAlO_4$	a=b=3.688 c=4.05	(1.327; 0; 1)	2.32
$SrNdGaO_4$	a=b=3.816 c=4.173	(1; 0; 1.847)	0.18

Table 2. Description of epitaxial relationships

Relationship	Substrate directions	Layer directions
1	[100], [010], [001]	[100], [010], [001]
2	[100], [010], [001]	[100], [001], $[0\bar{1}0]$
3	[100], [010], [001]	$[00\bar{1}]$, [010], [100]
4	[100], [010], [001]	[010], $[\bar{1}00]$, [001]
5	[100], [010], [001]	[001], [100], [010]
6	[100], [010], [001]	[010], [001], [100]



Misfit (upper) and epitaxial relationships mapping (lower) as the functions of substrate orientation ((001)-centered stereoprojections).