DIFFUSE SCATTERING IN MULTILYERS : a tool for the study of interfaces defects and disordered alloys

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Diffuse scattering of X rays is a particularly useful tool for studying interface and surface defects in single layer films. We have extended this technique to the study of metallic multilayers. X-ray diffraction measurements were carried out using a 4-circle diffractometer high resolution goniometer at the D23A anomalous dispersion beamline at the DCI synchrotron (LURE, Orsay). The use of both specular and off-specular measurements has provided probes of the samples structure in the vertical (growth) direction, and in the horizontal (parallel to interfaces) direction.

Small angle specular simulations: To perform the small angle specular simulations, we employed the matrix method technique of Vidal and Vincent [1] for calculating the specular electric fields at each interface of the sample. The diffuse scattering contribution at the specular condition was first removed from the data by subtracting the diffuse longitudinal scan having omega equal to $2\theta/2 + d\theta$, where $d\theta$ is small compared to θ. The advantages of high intensity and anomalous dispersion available with synchrotron radiation have greatly contributed to the quality of our data, for which the use of this simulation program has allowed a robust and precise extraction of several structural parameters, such as layers thicknesses and interfacial thicknesses "σ".

Small angle off specular simulations: To simulate the small-angles off-specular scans, we use the specular electric fields calculated at each interface of the samples, and then we apply the theoretical results of Daillant and Belorgey [2] for calculating the diffused scatterred intensity from these electric fields. The two additional structural parameters that can be extracted from these off-specular scans are the horizontal and the vertical correlation length of the interfacial roughnesses, $\xi(x)$ and $\xi(z)$ respectively. For za(x) and zb(x) being the vertical displacements (about average altitudes of z(0,a) and z(0,b) of two interfaces in the sample along the x direction, we supposed a gaussian profile of interfaces and defined our interface correlation function where (za(x)zb(0)) is equal to $\sigma(z,a)\sigma(z,b).\exp-(x/\xi(x))(x/\xi(x)).\exp-((z(0,a)-z(0,b))/\xi(z))((z(0,a)-z(0,b))/\xi(z))$ [3] [4]. The parameter $\xi(x)$ serves to distinguish interfacial roughness ($\xi(x)$ bigger than arround 1.5nm) from interfacial diffusion ($\xi(x)$ smaller than arround 1.5nm) [5].

Results: The samples are Mn/Ir(111) superlattices where Mn is pseudomorphic to Ir. Using a M.B.E. chamber in the 10(-10) vaccum range, we have grown three typical samples very similar with respect to period, relative thicknesses of Mn and Ir, and number of bilayers. The only parameter very different from one sample to the another one is the growth temperature: either room temperature, 373K or 573K. The small angle measurements and simulations show clearly that the interfaces of the superlattice grown at RT are poorly correlated ($\xi(z)$ is close to 15nm) and rough (σ varies from 0.7 to 1.1 nm from the bottom to the top of the sample, $\xi(x)$ is close to 20nm), and that the superlattice grown at 573K has rather well correlated ($\xi(z)$ is close to 20nm) and interdiffused (σ varies from 1.7nm to 1.3nm from the bottom to the top of the sample, $\xi(x)$ is close to 2nm) interfaces. The superlattice grown at 373K presents intermediate structural properties, with less disorder (σ varies from 0.3 to 0.8nm from the bottom to the top of the sample, $\xi(x)$ is close to 5nm, $\xi(z)$ is close to 15nm). All these structural results have been confirmed by transmission electron microscopy. Moreover, we show that large length-scale interfacial roughness is mainly due to the formation of terraces during growth at low deposition temperature, whereas small lengh-scale interfacial roughness occurs preferably at high

deposition temperature and is mainly due to an atomic interdiffusion (i.e. formation of an interface alloy) which manages to maintain a high degree of crystallographic order [6].

At the present time, we want to extend our technique to the study of disordered alloys. Then, we have produced pseudomorphic =46e(x)Mn(1-x)/Ir(100) superlattices having different stoichiometries (x varies from 0.8 to 0.3) [7]. The alloy crystalline structure is body centered tetragonal with a c/a ratio between 1.18 and 1.26. Our goal is to describe how a disordered alloy in the layers modify the specular and the off-specular intensity. We will also use the anomalous signal available on synchrotron radiation to distinguish Mn and Fe disorder.

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