A.6: Sc/Mg multilayer for soft x-ray emission spectroscopy applications

Soft x-ray emission spectroscopy technique provides information about density of occupied states and unfolds details of chemical and electronic properties of materials. Such spectrometers are designed using large *d* natural crystals and reflection gratings. Natural crystals such as Potassium Acid Phthalate (KAP) have *2d* periodicity of 2.663 nm and therefore can be used to cover photon energy in the 500-1500 eV region. The photon energy region below 500 eV requires a grating or artificially grown multilayer dispersive elements having the desired periodicity. Below the scandium *L*-edge region (400 eV), the Sc/Mg multilayer shows very good reflectivity performance and therefore is a promising optical element for scanning emission spectroscopy applications. Optimization of this multilayer system having a periodic layer arrangement of Sc 3 nm / Mg 3 nm with N = 25 layer pairs gives a reflectivity of ~60% below the 400 eV region at a 15° incidence angle, as the calculated results are shown in Figure A.6.1.

An extensive study on Sc/Mg based multilayer systems was carried out at the soft x-ray reflectivity beamline, BL-03, Indus-2, as a part of a Ph. D. thesis work titled: *"Interface analysis of nanoscale thin films"* submitted and defended at the Sorbonne University, Paris, France. The work included soft x-ray reflectivity and resonant reflectivity studies of bilayers, trilayers, and quadrilayers of Mg, Sc, and ZrC materials. The study of interface analyses provided vital information for the fabrication of multilayer mirrors to achieve ultra-smooth interfaces and, in turn, high reflectivity performances.

Near the absorption edges, the refractive index is sensitive to chemical environment. Any change in the local environment of the atoms affects the optical properties of the materials. The resonant soft x-ray reflectivity (SXR) technique was used to obtain elemental sensitive information by tuning the energy of x-rays to the absorption edges of Sc. The SXR fitted and measured curves of the Sc/Mg bilayer at different photon energies around the Sc *L*- absorption edge are shown in Figure A.6.2. The x-ray reflectivity data are fitted using a four-layer model comprising a top layer formed due to surface oxidation, an intermixed MgSc interlayer, the Sc layer, and an interlayer at the scandium and silicon substrate interface region. The δ-profile obtained from x-ray reflectivity analyses is plotted in Figure A.6.3. The fit reveals the formation of an interface layer on the Mg-on-Sc interface. The Sc layer is mostly uniform, with a density close to that of the bulk. An increase in the δ-profile (refractive index $n = 1-\delta+i\beta$) is seen at the Sc-on-Si interface, corresponding to the formation of a dense interlayer at the Sc/substrate interface region. The work covers detailed characterization of multilayers, bilayers, and trilayers of Mg, Sc systems using x-ray reflectivity and other techniques.

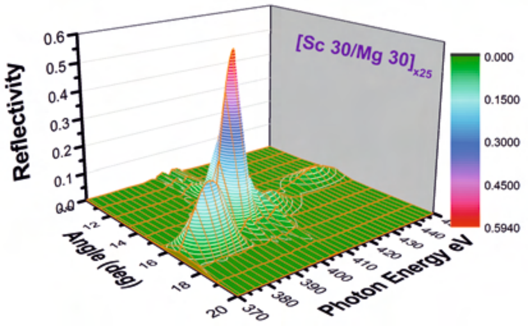

Fig. A.6.1: Calculated soft x-ray reflectivity of the Sc/Mg multilayer near the Sc L- edge region.

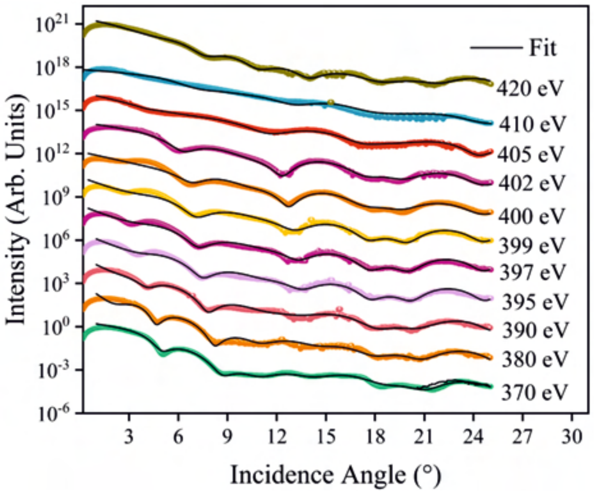

Fig. A.6.2: Measured and fitted angle-dependent SXR curves of the Mg/Sc bilayer at photon energies near the Sc L- edge.

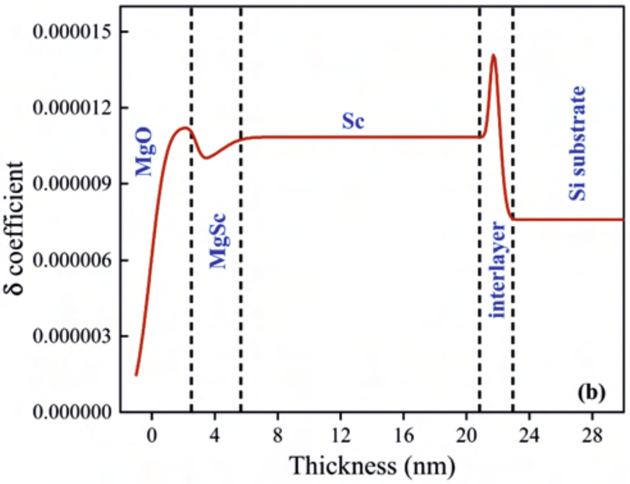

Fig. A.6.3: An in-depth δ-profile of the Mg/Sc bilayer obtained from the fit of x-ray reflectivity data.

For further details please refer: *Hina Verma et al., Thin Solid Films 763, 139595 (2022).*

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