# Thin Films and Coatings

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## Characterization of CrN films on MgO (100) by advanced TEM

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CrN has – besides its application as wear-resistant coating – recently gained considerable interest due to its unique antiferromagnetic configurations for which it has been used as a prototype material for strong magnetostructural interactions. This has recently led to numerous experimental and theoretical studies [1-3].

The CrN films in this work were deposited by d.c. magnetron sputtering of a Cr target at a constant total pressure of 1 Pa. The microstructure of two different CrN thin films grown (i) as a single layer at -40 V bias voltage, a target power of 6 kW and a temperature of 350 °C with a thickness of 1.4 µm and (ii) as a bi-layer with a thickness of 10 nm with a 10 nm-thin Cr top layer grown at -80 V bias, a target power of 2 kW and a temperature of 500 °C was investigated by transmission electron microscopy (TEM). The chemical analysis was carried out by electron energy-loss spectroscopy (EELS). Conventional TEM was performed by a Philips CM12 at 120 kV. High-resolution TEM (HRTEM) investigations and EELS analyses were conducted on a TEM/STEM JEOL 2100F at 200 kV equipped with an image-side $C_S$-corrector (CEOS) and an energy filter (Tridiem, Gatan). Geometric phase analysis [4] was carried out to analyze the relative strain across the interface. TEM specimens were prepared by a standard procedure, mechanically ground and polished and then thinned from both sides till perforation by $Ar^+$ ion milling using a precision ion polishing system of Gatan (Model 691).
While a thin Cr(10 nm)/CrN(10 nm) bi-layer grew with a single crystalline microstructure, the CrN single layer with a thickness of more than 1 µm forms as a polycrystalline film with a columnar microstructure on MgO substrate. $C_S$-corrected HRTEM studies revealed that both layers were grown epitaxially on the MgO substrate at the initial stage. Interfacial misfit dislocations at the CrN/MgO interface were observed and detailed atomic structures at the interface are revealed. The geometric phase analysis across the CrN/MgO interface revealed strain changes from -14.7% to +16.6% with respect to the unstrained MgO lattice due to the presence of misfit dislocations. In two-dimensional relative strain maps the strain fields of pure edge type dislocations show a symmetrical shape with compressively stressed and stretched regions in x-direction and strain-free structure in y-direction (see centered dislocation in Figure 1). The map was calculated using the 111 and 200 reflections (Figure 1d).

In addition to the structural characterization, detailed EELS analysis was performed for the CrN single layer across the interface. The EEL spectra recorded at or close to the film-substrate interface (Figure 2a) show the evolution from the CrN film to the MgO substrate. This is reflected by a gradual change of the O-K, N-K and Cr-$L_{2,3}$ edges when crossing the interface. Because of the overlapping of the Cr-$L_{2,3}$ with the O-K edge, the multiple linear least-squares (MLLS) fitting was applied to the data to map out the respective Cr and O signals. A spatial distribution of the CrN and MgO components is shown in Figure 2b. It further reveals an interface width (from CrN to MgO) of about 4.3 nm.

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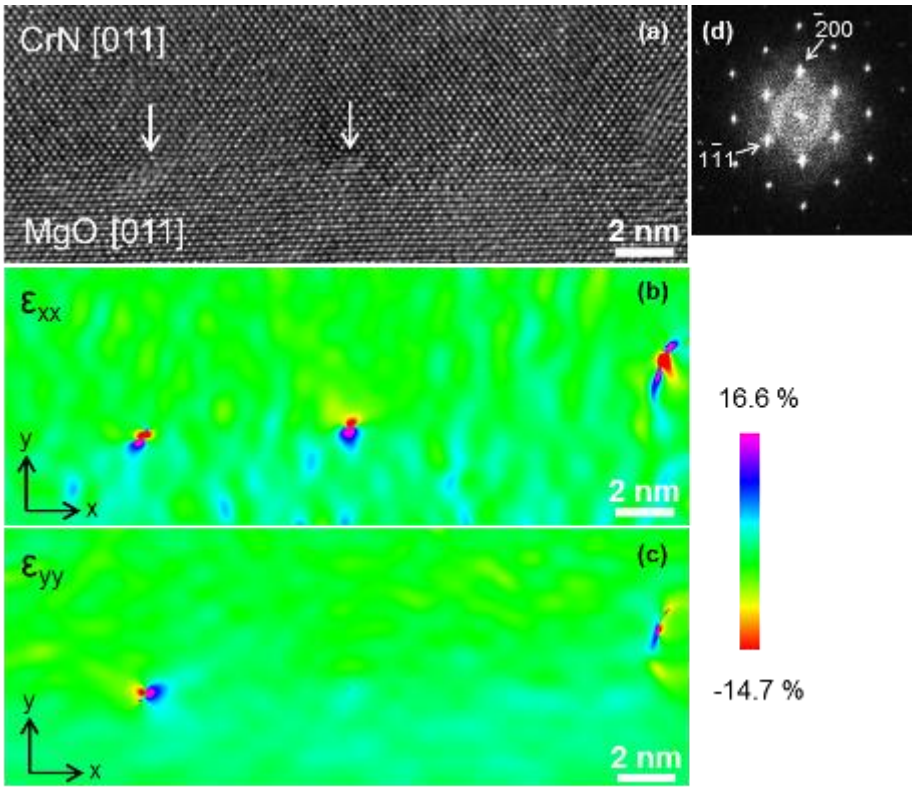


**Figure 1:** a) HRTEM image of the CrN/MgO interface of the bi-layer sample; b) relative strain map in x-direction and c) y-direction; d) power spectrum with selected reflections.

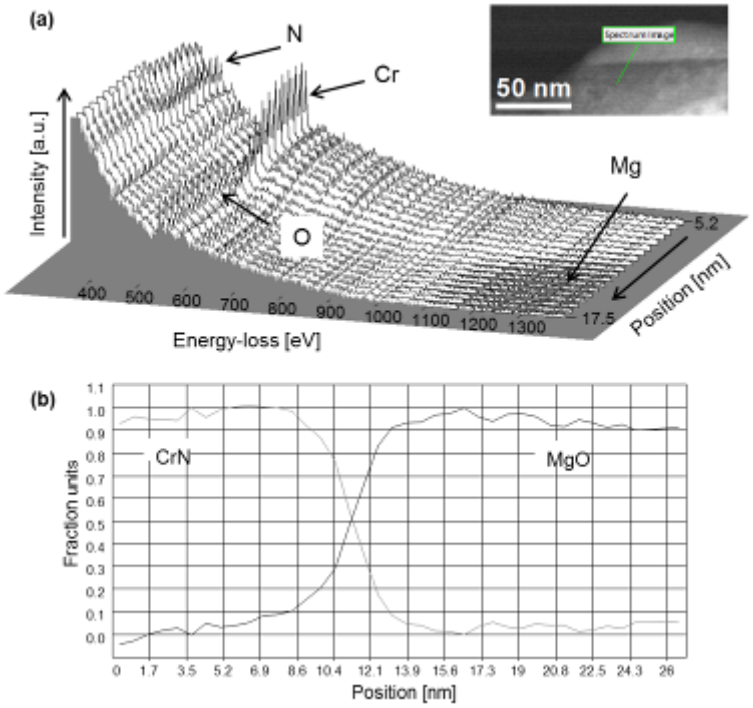


**Figure 2.** a) A section of line scan spectra at or close to the CrN/MgO interface with corresponding STEM image. The position of the spectra corresponds to the b) spatial distribution of the two components (CrN film and MgO substrate) across the interface obtained by MLLS fitting