



FeO(111) ULTRA-THIN FILM STRUCTURE INVESTIGATION

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Abstract – Iron monoxide has been synthesized by evaporation ⁵⁷Fe in UHV and oxidation (10^{-7} - 10^{-6} mbar O₂). The FeO ultra-thin films prepared on Ag(111), Ni(111) and Pd(100) were studied by means of XPS, Mössbauer spectroscopy (CEMS) and LEED. The surface structure was determined using a quantitative approach of the LEED data.

The synthesis of transition metal oxide films with single phases represents a challenge in surface science and can reveal important physical properties, especially in the ultra-thin film regime. In comparison to magnetite and hematite, iron monoxide has been much less investigated, since FeO is not as stable at ambient conditions. At ambient pressure and low temperature bulk-FeO adopts a distorted B1 structure (rhombohedral strain) due to the antiferromagnetic ordering of Fe²⁺ moments in hexagonal planes stacked along the [111] direction of the crystal. Above the Néel temperature (T>198K) a cubic rocksalt structure is observed. At high temperatures and pressures (p>120GPa and T>1000K), FeO transforms from the rhombohedrally distorted B1 phase to a NiAs (B8)-anti-NiAs (iB8) superlattice. Very little is known about this system in ultra-thin film form, and even less about the substrate influence.

In this work the growth of iron monoxide onto Ag(111), Ni(111) and Pd(100) substrates is investigated. The preparation of the FeO films has been carried out under ultra-high vacuum conditions by repeated cycles of electron-beam evaporation of high purity ⁵⁷Fe and oxidation in (10^{-7} - 10^{-6} mbar)-O₂ partial pressure. Several combinations of evaporation rates, oxygen pressure, and annealing procedures were tested, in order to establish the best conditions to prepare films with a high concentration of FeO. Chemical composition and phases were determined by X-ray Photoelectron Spectroscopy (XPS) and Conversion Electron Mössbauer Spectroscopy (CEMS). Low Energy Electron Diffraction (LEED) data were collected in order to determine the surface structure. The SATLEED code by M. A. Van Hove was used to model the I(V)-LEED theoretical curves of the FeO(111) surface. A previous work of our group on the FeO(100) system [1] has revealed its structure to be bulk-like (B1 structure). We have modeled the B1 structure for the (111) surface as well, but that has not matched our experimental I(V)-curves. For that, several stacking sequence of close-packed planes were tried. The best reliability factor was obtained for an oxygen terminated structure with a combination of B1 and B8 structure (CbAcAb stacking sequence).

[1] E. Lopes, G.J. P. Abreu, R. Paniago, E. A. Soares, V.E de Carvalho, H.-D. Pfannes, Surface Science **601** (2007) 1239-1245.