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# On the conductive properties of MgO films grown on ultrathin hexagonal close-packed Co(0001) layer

L. Gladczuk *, M. Aleszkiewicz

*Institute of Physics, Polish Academy of Sciences, al. Lotnikow 32/46, 02-668 Warsaw, Poland*

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ABSTRACT

Here we present a scanning tunneling microscopy study of electrical conductivity of (110)-oriented MgO ultrathin films grown on hexagonal close-packed Co(0001) surface by molecular beam epitaxy, being a good candidate for tunneling barrier for future-generation spintronic devices. Three-dimensional growth of the tunneling barrier, expected for compressive strains emerging at the Co/MgO interface, is demonstrated by reflection high-energy electron diffraction and atomic force microscopy. The 5 eV height of the full barrier of MgO is reached at a layer thickness of 4 nm. Thinner MgO layers exhibit randomly distributed spots of the high conductance on the tunneling current map. The current–voltage curves indicate the existence of vacancies in MgO crystal lattice, lowering the resistivity of the tunneling barrier.



## 1. Introduction

Spin-dependent tunneling of electrons between two magnetic films separated by an insulating layer (tunneling barrier) strongly depends on the structural and electronic properties of the electrodes and barrier material, as it has been revealed by theoretical and experimental studies [1–11]. Improvement in the material and interface quality results in an enhancement of the relative change in resistance values which describe the quality of the entire junction. First-principles calculations have predicted that the crystalline tunnel barriers may give rise to high spin polarization and tunnel magnetoresistance (TMR) values because of the occurrence of a strongly spin-dependent evanescent decay of specific wave-functions, with particular transverse momentum values, across the tunnel barrier [12]. Numerical studies for perfectly (100)-oriented Fe/MgO/Fe magnetic tunnel junctions (MTJs), have suggested almost ten-fold enhancement of TMR values for sufficiently thick MgO tunnel barriers [4,7]. Very large magnetoresistance values have been estimated for epitaxial MTJs [4,7,13,14]. However, at the present stage, it is difficult to assume whether the epitaxial structures would be used in devices, but definitely they can be employed as an outstanding model system for investigation of the spin-dependent phenomena and the evolution of devices on the basis of theoretical calculations.

Recently, several groups have reported pseudo-epitaxial MgO layer growth on Co. However, the details of surface morphology and conductive properties are not well understood [9]. It is possible that the interfacial transition-metal oxide layer which is crucial for Fe(100)/MgO(100) growth can be omitted in the case of body-centered cubic Co(100)/MgO(100) or FeCo(100)/MgO(100), what means that these heterostructures would become easier to grow [7].

Despite the high value of the bulk magnesium oxide band gap of 7.8 eV, the MgO thin films are characterized by sufficiently high conductivity to be imaged with scanning tunneling microscopy (STM). Therefore, the STM studies, performed under appropriate bias conditions, may provide direct information on morphology and electronic structure of defects in studied oxide films [15].

In this study, the influence of the MgO layer thickness in the MgO/Co(0001) bilayer on the tunneling barrier height is examined. Strong anisotropy of the hexagonal close-packed (hcp) Co(0001) films leads to the perpendicular magnetization in sufficiently thin Co layer, what is of considerable interest for their applicability in MTJ devices. It is demonstrated that in the MgO layer with a suitably smooth surface and reasonably high thickness, randomly distributed spots of higher conductivity appear due to the defected crystal lattice.

## 2. Sample preparation and characterization

Heterostructures of Mo/Au/Co/MgO with various MgO layer thickness were grown on sapphire using the molecular-beam epitaxy. Molybdenum, cobalt, and magnesium oxide were deposited by an electron-gun vapor source, and gold was thermally evaporated from a standard Knudsen cell. Initially, a 20 nm thick Mo seed layer was deposited on $Al_2O_3$ substrate, heated up to 950 °C, and after cooling down a Au buffer layer (20 nm) was grown. Subsequently, the structures were annealed (30 min at 200 °C), and the Co (1 nm) magnetic film followed by MgO layer of the desired thickness were deposited at ambient temperature. The growth characteristics of this type of heterostructures had been already described in detail [16].

* Corresponding author. Tel.: +48 22 843 66 01x3110.
*E-mail address:* gladl@ifpan.edu.pl (L. Gladczuk).

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In this study the structure and chemical composition of the samples were characterized during growth by reflection high-energy electron diffraction (RHEED), (Staib, EK-12-R, 12 keV electron beam) and Auger electron spectroscopy (AES), (OCI, BDL600IR). The first derivative of AES spectra was recorded using a 3 keV electron beam at 30 mA and modulation voltage of 10 V. The post-growth characterizations; i.e., surface morphology and magnetic properties of the cobalt layer, were performed using atomic force microscopy (AFM), STM, and magnetic force microscopy (MFM) with MultiMode scanning probe microscope. AFM was operated in dynamic mode (tapping mode) using silicon tips (Olympus; AC160TS; spring constant 42 N/m, resonance frequency 300 kHz). STM images were obtained with precision-cut wire Pt–Ir tips (Bruker; model PT) operating at picoampere-range currents. For MFM characterization the low moment magnetic tips were employed (Nanosensors; LM-MESP; 2.8 N/m, 75 kHz). The tip was magnetized along its axis prior to imaging and MFM images were taken in dynamic mode with resonant frequency shift detection, using LiftMode operated with 10–100 nm lift heights.

## 3. Results and discussion

### 3.1. Morphology

Possible atomic arrangement between Co and MgO layers and the resulting reconstruction of the interface plane is schematically shown in Fig. 1. Obviously, the (111) planes of MgO provide the best matching crystal orientation, since the Co surface exhibits hexagonal symmetry. The interface consists of hcp Co(0001) triangles with side length $d_{Co\text{-}Co} = 0.251$ nm and the Mg or O triangles with side length $d_{O\text{-}O} = 0.298$ nm. The MgO[110] vector is parallel to Co$\left[2\ \bar{1}\ \bar{1}\ 0\right]$ direction. In each corresponding cell, one O or Mg atom binds above a surface Co atom. At room temperature, in the case of perfect lattice matching between Co and MgO, MgO is under large, (15%), compressive strain. The RHEED patterns of 1 nm films: Co $\left[0\ 1\ \bar{1}\ 0\right]$, Co$\left[2\ \bar{1}\ \bar{1}\ 0\right]$, MgO [112], and MgO[110] are shown in Fig. 2. The streaked RHEED pattern which is characteristic for terraced surface suggests that the MgO film grows via a three-dimensional (3D) or islanding process. The resulting microstructure is not surprising for the [111] growth direction on rocksalt-type plane, since it is not easy to accomplish a smooth layer-by-layer growth. For MgO, the relatively low surface energies give rise to an instability of the (111) reconstruction with respect to (100)—the ratio of the (111) to (100) surface energy is 1.29 only [17]. Moreover, a rough or grainy morphology is expected, because of the large lattice mismatch between magnesium oxide and cobalt. We found that the distances between Mg or O atoms calculated from the streak positions observed in the RHEED images are $d_{[112]} = 0.144$ nm and $d_{[110]} = 0.260$ nm, whereas the distances for cobalt are $d_{[0\ 1\ \bar{1}\ 0]} = 0.136$ nm and $d_{[2\ \bar{1}\ \bar{1}\ 0]} = 0.232$ nm, respectively. The strains are reduced with increasing thickness of the MgO film and the thickness of 1 nm is large enough to obtain fully relaxed MgO layer.

A representative example of the surface morphology of the 1 nm Co film examined by AFM is shown in Fig. 3a. The Co crystallites form atomically-flatly topped terraces of about 100 nm width and separated by atomic steps of sub-nanometer height. The height of the terraces (i.e. the vertical distance on the steepest parts of the profile line in Fig. 3a) corresponds to the height of two Co(0001) atomic layers. The distances between the histogram peaks calculated for plane-fitted 500 × 500 nm$^2$ image are 0.205 nm and 0.41 nm, what corresponds to 1 monolayer (ML) and 2 MLs Co terrace height, respectively, as shown in the inset of Fig. 3a. The roughness parameters for the 500 × 500 nm$^2$ surface area are: root mean square (RMS) roughness - 0.146 nm; Ra (mean roughness) - 0.114 nm; max. height (maximum vertical distance between the highest and lowest data points in the image) - 1.120 nm. This type of epitaxial growth of cobalt films on Au is known and is induced by the strains at the Au(111)/Co(0001) interface [18].

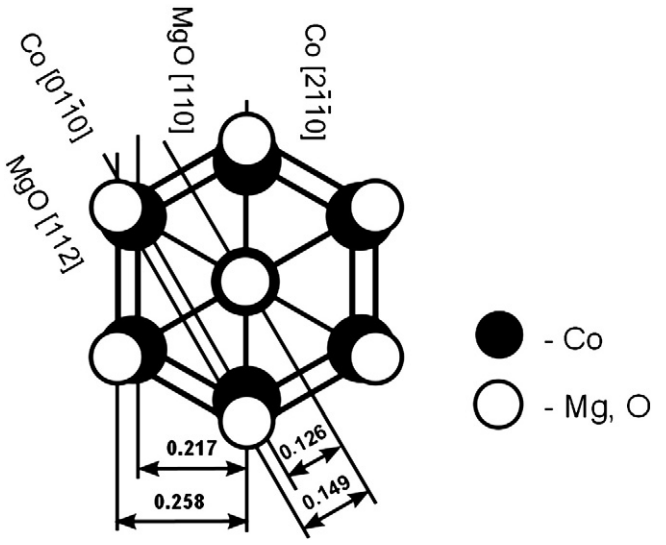


**Fig. 1.** Closely matched atomic positions of the hcp Co (0001) plane (full circles) and bcc MgO (111) plane (open circles). All distances are in nanometers.

The AFM image of the 1 nm thick MgO layer surface shown in Fig. 3b, demonstrates again a grainy microstructure with features of 100 nm diameter similar to underlying Co. The step height at cross-section line in Fig. 3b corresponds to the Mg–O layer distance ($d_{[Mg\text{–}O]} = 0.260$ nm) in a [111] direction. The average height of a single terrace estimated as above (i.e., as the separation of the peaks at the height histogram calculated for plane-fitted 500 × 500 nm$^2$ image) is close to the double Mg–O layer distance in [111] direction (inset in Fig. 3b). The values of RMS roughness are larger by 10% than those for Co while the maximum vertical distance remains unchanged (RMS 0.164 nm; Ra 0.131 nm; Max. height 1.195 nm).

The grain size is enlarged with increasing the MgO layer thickness, as is seen in Fig. 3c, where the 4 nm thick MgO layer surface image is presented. The surface roughness parameters decrease to the values similar to those of Co layer (RMS - 0.146 nm; Ra - 0.117 nm) except of vertical range, where the max. height is smaller than that for Co (max. height 0.951 nm). The separation of the two distinct peaks at the height histogram is 0.520 nm (inset of Fig. 3c). There is another less pronounced peak between them, suggesting that the distance of 520 nm represents 2 ML terrace height. The MgO steps of 1 ML (~0.260 nm) and 2 MLs (~0.520 nm) height can be also recognized at the line profile (bottom of Fig. 3c).

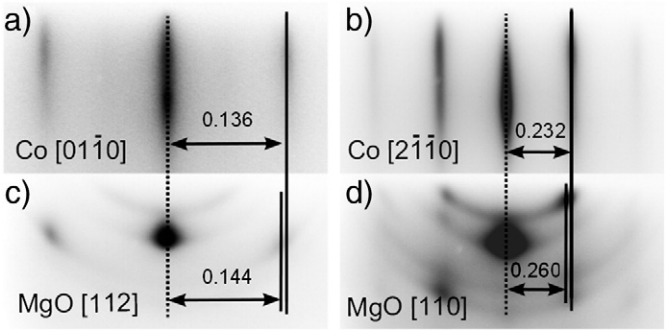


**Fig. 2.** The RHEED patterns of 1 nm films collected along the plane crystallographic direction: a) Co$\left[0\ 1\ \bar{1}\ 0\right]$, b) Co$\left[2\ \bar{1}\ \bar{1}\ 0\right]$, c) MgO[112] and, d) MgO[110]. All distances are in nanometers.