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Structure of epitaxial Fe films on MgO(100)

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Abstract

We investigated the epitaxial growth of bcc Fe on MgO(100) using STM and LEED as a function of growth temperature. We found the island size and shape to vary with the deposition temperature and post-deposition annealing. Relatively smooth island surfaces can be obtained by deposition around 160°C, however, the island heights distribution is rather irregular then. The rms roughness is lowest for deposition at 110°C. At lower deposition temperatures the islands become more round-shaped, likely due to a reduction of step edge diffusion. Post-deposition annealing to temperatures around 210°C increases the overall variation of the island height distribution.

Keywords: Thin films – epitaxial; Structure; Film growth; Scanning tunneling microscopy

1. Introduction

Thin magnetic layers often show a variety of properties different from the bulk material. Usually, the magnetic properties of such films strongly depend on their structure on the atomic scale as well as their morphology.

We investigated the epitaxial growth of bcc Fe on MgO(100). This material combination is particularly interesting for several reasons. First, it allows the epitaxial growth over a wide range of Fe thickness since the bcc Fe lattice fits onto the fcc MgO lattice with a mismatch of 3.5% following the epitaxial relationship Fe(100)[011]/MgO(100)[110]. Secondly, the Fe monolayer on MgO is predicted to have unique magnetic properties [1] which makes it interesting to explore the possibility of growing ultrathin flat Fe layers on this substrate. Additionally, the Fe(100) surface shows a highly spin-polarised surface state [2] which can be studied by STM spectroscopy. The existence of this surface state makes such Fe layers an interesting test sample for spin polarised tunneling experiments. Finally, the structural properties of Fe/MgO are decisive for the amplitude of the giant magnetoresistance of epitaxial Fe/Cr superlattices grown on MgO [3]. A technical drawback, however, is the lack of conductivity of the substrate which impairs STM and LEED studies.

In this contribution we will present the growth morphology of epitaxial Fe films on MgO(100) studied by scanning tunneling microscopy (STM) and low energy electron diffraction (LEED). Results are shown for films up to 30 Å thick, for growth temperatures (T_g) in the range from 0 to 200°C.

2. Experimental

The experiments have been performed in a UHV MBE system for surface analysis. The base pressure is 3×10^{-11} mbar, the pressure during evaporation about 3×10^{-10} mbar. The sample temperature is measured by averaging the read-out of two thermocouples attached to the sample holder on either side of the sample and an infrared pyrometer. Details of the system are described elsewhere [4].

The cleaved and polished MgO(100) single crystalline substrates had a typical size of 1 cm^2. An investigation of the surface with AFM in air showed large flat areas (typically > 1 μm in diameter) separated by atomic steps. In order to provide electrical contacts to the to be grown films contact pads of Au have been deposited along two edges of the substrate surface. The clips of the sample holder system pressing on these pads will connect them to ground. The pads have been found to resist the later treatment of cleaning and heating without Au diffusing across the surface and to make ohmic contacts to the thin films. However, still electrical contact to the Fe films is only provided if the films are continuous rather than consisting of separated islands. This allows a simple proof of the continuity of the films for the different growth temperatures.

The MgO(100) single crystal substrates were then cleaned several times in acetone, hexane and isopropanol. After introduction into the UHV chamber the substrates were heated several times up to 1150°C. After this treat-

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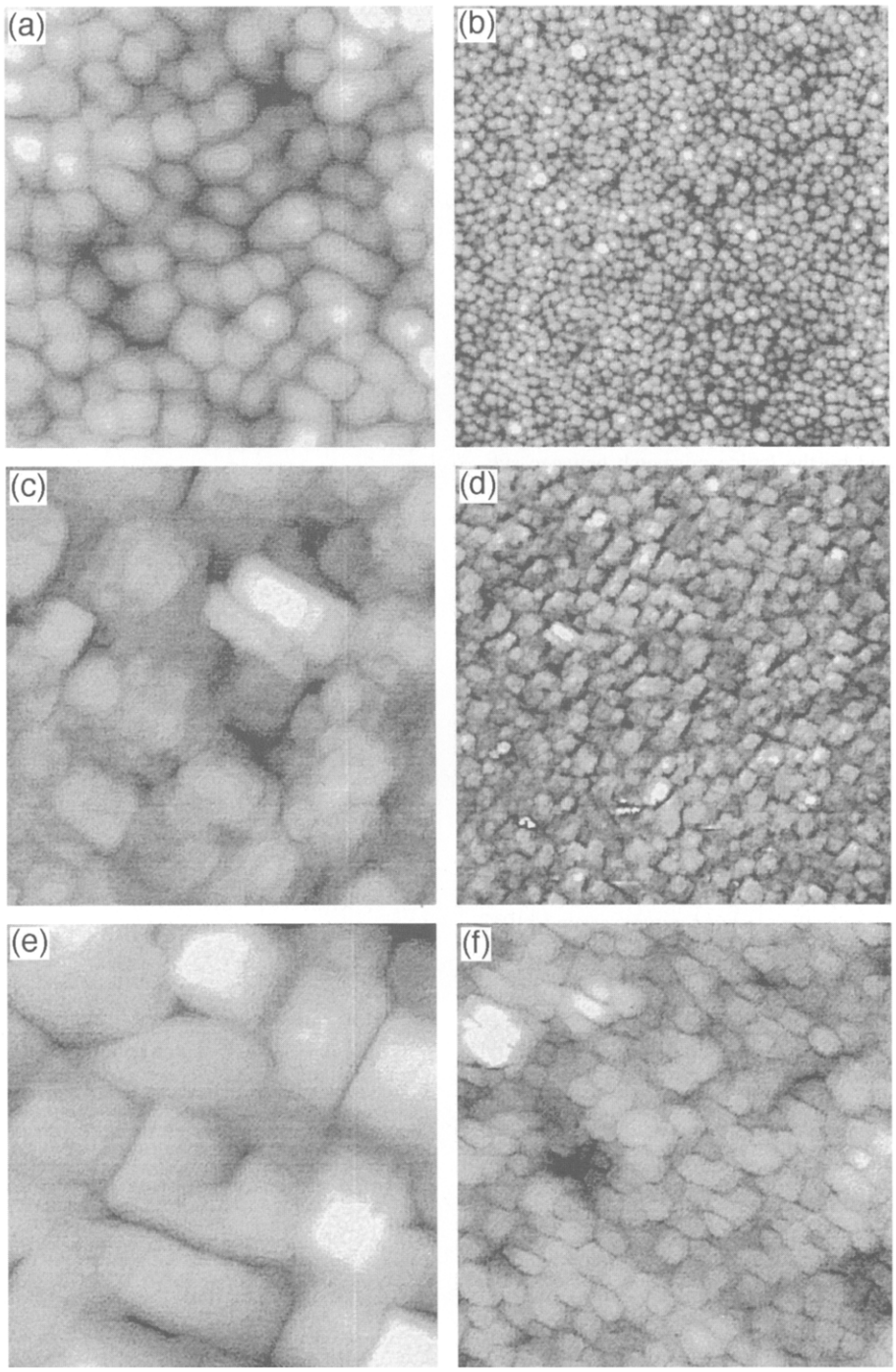

Fig. 1. STM images of 20 Å (a, b, c, d) or 30 Å (e, f) Fe deposited on MgO(100) at different temperatures $T_g = 20°C$ (a, b), 110°C (c, d) and 160°C (e, f), respectively. Scan sizes: 50 nm × 50 nm (a, c, e) and 200 nm × 200 nm (b, d, f). The z-range from black to white is respectively 25 Å (a), 50 Å (b, e, f), 15 Å (c) and 20 Å (d). The pictures were taken with 85 pA tunnel current and respectively: −140 mV (a), 10 V (b), −243 mV (c), −80 mV (d) and −1.33 V (e, f) bias voltage. The rms roughness and the typical island diameter are respectively 1.8 Å, 50 Å (a, b), 1.3 Å, 100 Å (c, d) and 7 Å, 120 Å (e, f).

ment only traces of carbon could be detected on the surface using Auger electron spectroscopy. The ratio between the Mg and O intensities, however, remained unaltered, indicating the absence of important changes in the surface stoichiometry. The deposition rate of the Fe was typically 1 Å/min.

3. Results

All of the Fe films discussed here showed a LEED pattern corresponding to the epitaxial relationship Fe(100)[001]/MgO(100)[011]. The heights of the atomic steps on the Fe films in the STM images (when visible) correspond to the bulk lattice constant. The limited resolution, however, did not allow to distinguish small deviation from the undistorted bcc lattice. From X-ray diffraction measurements it is known that Fe films grown under these conditions have a small (about 1%) contraction of the vertical lattice constant to compensate for the in plane expansion imposed by the lattice mismatch between substrate and film [5].

In Fig. 1 are shown large- and small-scale STM pictures taken under the conditions given in the caption. The room temperature deposition yields round shaped islands (Fig. 1a, b) with a typical diameter of 50 Å (Fig. 1a). The shape and high nucleation density is likely caused by the reduced mobility for diffusion along step edges at these temperatures. Increasing T_g to 110°C (Fig. 1c, d) leads to square shaped islands with an increased typical diameter of about 100 Å. At the same time the rms roughness decreases. At even higher T_g (160°C) the rms roughness increases again due to an increased jaggedness of the islands heights distribution (Fig. 1f). The surfaces of the individual islands, however, become more smooth with monoatomic steps being visible (Fig. 1e).

Post-deposition annealing to temperatures around 210°C increases the overall island height distribution and increases the size of the terraces on top of the islands. A deposition at such temperatures yielded non-continuous films at these thicknesses.

4. Discussion

Varying the growth conditions it is possible to produce epitaxial Fe films on MgO(100) with a large variety of island shape, size and flatness. This is certainly a well-suited play ground for studies of the surface states of Fe and their possible magnetic polarisation. Such properties strongly depend on the local arrangement of the atoms, thus island size, terrace width and straightness of the step edges will play a crucial role. The possibility for growing large scale monoatomic thin Fe layers on MgO(100) must be assessed pessimistically. Besides possible complications due to intermixing at the Fe/MgO interface and the exact atomic positions, this study shows that it will be difficult to produce films of the required homogeneity. Perhaps changes in the growth kinetics at growth temperatures below room temperature will improve the properties. In the framework of Fe/Cr superlattices showing the Giant Magnetoresistance the step density seems to play a decisive role for the amplitude of the effect. However, in order to establish the antiferromagnetic arrangement of the magnetisation directions of adjacent Fe layers, strong fluctuations in the layer thicknesses have to be avoided. The best conditions will probably be met at T_g around 100°C where the islands a rather uniform in their average height but show a large step density.

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