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A LEED study of surface relaxation in Fe(1 1 0) epitaxial film on W(1 1 0)

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ABSTRACT

The near-surface structural properties of epitaxial Fe(1 1 0) films on W(1 1 0) were studied using quantitative low-energy electron diffraction analysis. A discernible, up to 1%, relaxation of the outermost atomic layers was found, in contrast to the bulk Fe(1 1 0) surface, which shows almost no relaxation.

1. Introduction

Fe(1 1 0) epitaxial films on W(1 1 0) represent a prototype system for studying structural, electronic and magnetic properties, which are dependent on the growth mode, film thickness and temperature and are determined by the surface and interface. Ranging from a pseudomorphic Fe monolayer on W(1 1 0) [1] and ultrathin films [1,2] to Fe(1 1 0) film surfaces that mimic bulk Fe-surface properties [3], this system is one of the most intensely investigated systems in surface science. The growth of Fe/W(1 1 0) has been investigated by low-energy electron diffraction (LEED) and Auger electron spectroscopy (AES) [1] and by scanning tunnelling microscopy (STM) [2,4,5]. It is generally accepted that the first Fe monolayer (ML) grows pseudomorphically on W(1 1 0) despite a large misfit of 10%. For higher coverage, between 1.5 ML and 2 ML, the formation of misfit dislocations has been observed [1,2], and for ultrathin films (>2 ML), satellite spots arranged in diamond-shaped groups appear around the integer-order reflections of the W(1 1 0) substrate. This long-range ordered misfit-dislocation network, which is usually localised close to the W–Fe interface, relieves the strain induced in the growing adlayer due to the lattice constant difference between the tungsten substrate ($a_W = 3.16$ Å) and the bulk iron ($a_{Fe} = 2.86$ Å). The misfit dislocations cause a lattice distortion, which is projected to the film surface, and can be observed as satellite spots in the LEED pattern [1] and as vertical corrugations forming a three-dimensional dislocation network in STM images [2]. In wedged-shaped Fe islands on W(1 1 0), STM has revealed such a surface modulation for Fe films as thick as 11 ML [2]. A detailed quantitative surface X-ray diffraction (SXRD) analysis produced a complex picture of Fe film distortions for films as thick as 13 ML, showing a two-dimensionally modulated structure in which the modulation amplitudes inside the film decrease with increasing distance from the interface [6]. The average Fe structure has been interpreted as a slightly laterally distorted bct phase.

The complex film structure is reflected in magnetic properties such as perpendicular magnetisation in the monolayer range and the spin reorientation transition (SRT) from perpendicular to in-plane magnetisation [7,8], with the in-plane easy axis direction differing from that of the bulk, i.e., [1 −1 0] instead of [0 0 1]. The unusual easy magnetisation axis arises from the competition between the magnetocrystalline volume, surface and strain anisotropies [9].

With increasing Fe thickness, the LEED superstructure is simplified, the satellite spots fade out, and the film appears to relax. Above a thickness of 20 ML, the surface layers are considered to be undistorted [3]. The surface of an Fe(1 1 0) film on W(1 1 0) for thicknesses ranging from 25 Å to 200 Å is assumed to represent the Fe bulk surface properties in many studies related to structural [10], chemical [11], electronic [12] and magnetic [13,14] properties.

Despite the bulk-like character of the surface geometry for films thicker than a few tens of monolayers, their magnetic properties can still deviate from the bulk properties, as represented by the unusual [1 −1 0] easy magnetisation axis. The bulk magnetisation direction is restored by increasing the film thickness above a certain

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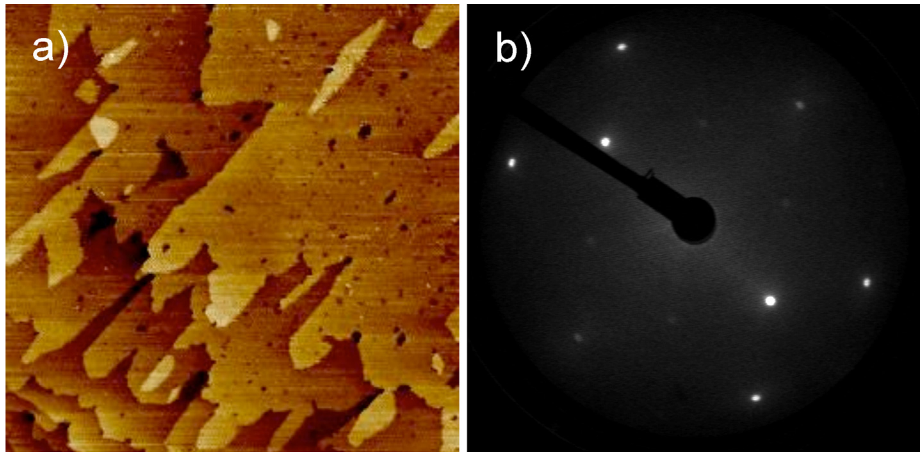

Fig. 1. STM image (a) and LEED pattern taken at an electron energy of 225 eV (b) for an Fe(1 1 0) film on W(1 1 0) deposited under the optimised growth conditions.

critical value defining the in-plane SRT [15]. The spontaneous magnetisation switching from [1 −1 0] to [0 0 1] with increasing thickness occurs through a complex scenario that depends on the film structure and morphology [16,17], and the critical thickness, depending on the preparation and measurement temperature, can vary over a wide range from 40 Å [18] to 200 Å [19]. Recently, this SRT transition was theoretically studied from a thermodynamic approach [20], and in agreement with experimental analysis [16], it was demonstrated that the explanation of the noncollinear magnetisation distribution requires a modification of the Fe film exchange coupling compared to the bulk.

Detailed studies on the surface structural properties of thick Fe(1 1 0) films on W(1 1 0) are rare. The (1 1 0) bcc-like surface structure is generally verified through qualitative LEED observations, and it has been demonstrated that optimised preparation conditions lead to sharp and background-free images, indicating a good surface quality [11–13,21].

The evolution of the thermo-elastic properties of epitaxial iron films on W(1 1 0) over a wide thickness range, from 1 ML to 45 ML, was analysed based on the phonon densities of states derived from the nuclear inelastic scattering of synchrotron radiation [21]. In this type of experiments only vibrations corresponding to in-plane displacements can be detected. For the thickest film investigated, phonon softening with respect to the bulk was observed, which may be attributed to lattice distortion. Similar surface-sensitive studies have shown that the vibration amplitudes of the surface atoms exceed the bulk value by 30%, in perfect agreement with DFT calculations [22].

The surface structure, including relaxation, determines fundamental properties such as lattice dynamics [23], electronic [24] and magnetic structure [25] and reactivity [26]. This fact motivated us to undertake a detailed study based on the experimental and theoretical analysis of quantitative LEED data (so-called IV analysis), which sheds some light on the Fe/W(1 1 0) film structure through a comparison with the bulk Fe surface [27], for which a negligible surface relaxation was reported. In contrast, the present study demonstrates a discernible variation in the near-surface atomic inter-layer spacing in Fe(1 1 0) epitaxial film grown on W(1 1 0) and demonstrates that epitaxial strains are present in films as thick as 4 nm.

2. Experimental details

The experiments were performed in an ultrahigh vacuum system (base pressure: 1×10^{-10} mbar) equipped inter alia with a metal deposition facility, a STM and LEED/AES optics (OCI Microelectronics). The Fe films were grown on a W(1 1 0) single crystal oriented within an accuracy of 0.1°. The crystal was thoroughly cleaned using a standard cycling procedure of annealing under an O_2 partial pressure of 1×10^{-7} at 1200 °C, followed by flash heating at 2000 °C, which resulted a background-free LEED pattern and a clean surface with only traces of carbon, as verified by AES. Iron was thermally evaporated from a BeO crucible at a rate of 2 Å/min, as controlled by a quartz crystal monitor. Optimum growth conditions for a flat surface with a thickness of 3–10 nm were realised by deposition at 100 °C followed by annealing at 500 °C. The resulting surface morphology is shown in Fig. 1a. The STM image reveals a surface characterised by terraces elongated in the [0 0 1] direction, which is typical for the Fe on Fe(1 1 0) homoepitaxy [10]. Pit defects decorating the surface are formed as a result of annealing and are most likely related to strain relief. A corresponding LEED pattern acquired at 225 eV is shown in Fig. 1b. For the IV measurement, the Fe film thickness was chosen as 4 nm. Such a film was thick enough to ensure a 1 × 1 LEED pattern while being thin enough for the surface layers to still be affected by epitaxial strains.

IV-LEED measurements of the diffracted beam intensities as a function of the electron energy were realised by collecting subsequent LEED images at 1-eV steps, in the energy range of 50–450 eV, using the nominally normal incidence geometry. The entire data acquisition process took several minutes.

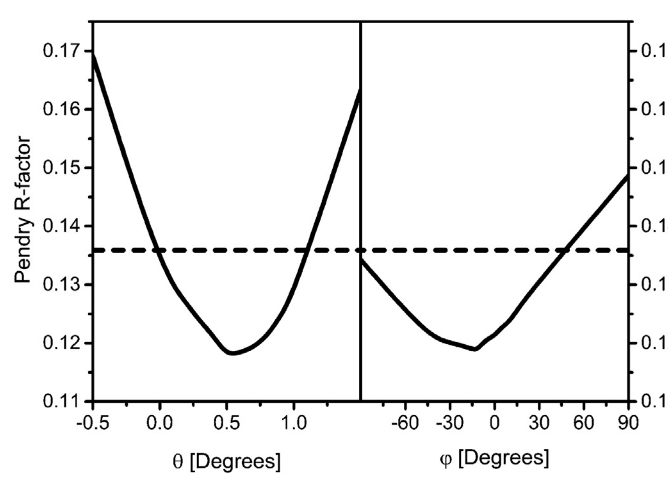

Fig. 2. Variation in the beam-averaged Pendry *R*-factor for the *IV* spectra, plotted as a function of incidence angle: polar θ and azimuth φ. The dashed horizontal lines indicate the R_{min} + Var(R_p) value, where R_{min} is the minimum value of R_p and Var(R_p) is the standard deviation of R_p calculated for all measured beams.