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**LETTER TO THE EDITOR**

# Quantitative analysis of scanning tunnelling microscope images of Fe grown epitaxially on MgO(001) using length-dependent variance measurements

S M Jordan, R Schad, J F Lawler†, D J L Herrmann and H van Kempen‡

Research Institute for Materials, University of Nijmegen, Toernooiveld 1, NL-6525 ED Nijmegen, The Netherlands

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**Abstract.** The roughness parameters of STM images of bcc Fe grown epitaxially on MgO(100) were analysed as a function of growth temperature in the range between 295 K and 595 K. The images were evaluated by means of length-dependent variance measurements revealing both vertical and lateral roughness information. The correlation length increased from 15 to 30 nm and the rms roughness decreased with increasing growth temperature whereas the fractal dimension remained constant.

The study of the roughness of growing crystals has long been of paramount interest from both scientific and technological perspectives. In particular, the behaviour of the growth front during thin-film deposition [1–7] is of particular relevance. The films' physical properties will very much depend on the smoothness or roughness of the final growth front which will form the interface to the adjacent material or the surface that interacts with the environment. For instance, the interfaces in field-effect transistors or tunnel junctions have to be extremely flat to guarantee homogeneous insulator thickness, whereas the so-called giant magnetoresistance effect in magnetic multilayers is enhanced by a certain degree of interface roughness. Proper control of the surface properties requires an understanding of the underlying growth mechanisms which can be achieved by detailed structure analysis of surfaces prepared under various growth conditions. The chosen system makes an ideal model, since it is displays interesting island formations, which change in structure with changing deposition temperature.

We have applied the method of length-dependent variance measurements to scanning tunnelling microscope images of epitaxial Fe(001) layers 5 nm thick grown on MgO(001) substrates at a rate of 0.13 nm per minute under ultrahigh-vacuum conditions at temperatures between 295 K and 595 K [8]. The substrate was prepared by solvent washing and subsequent heating in vacuum to 1070 K for one minute. This resulted in a KLL Auger C peak equivalent to 6% of one monolayer. AFM investigations showed that the MgO was of adequate flatness; single-atom-high terraces of widths up to 200 nm were seen. STM investigations of the completed films were then made *in situ* using a mechanically cut Pt–Ir tip.

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† Current address: School of Physical Sciences, Dublin City University, Ireland.

‡ Author to whom any correspondence should be addressed; telephone: 00 31 24 3653499; fax: 3652190; e-mail: hvk@sci.kun.nl.

The $(2+\epsilon)$-dimensional roughness of a self-affine surface was analysed for its length scale dependence using the height-variation function

$$g(L) = 2\sigma(L)^2 = \langle [z(r) - z(r')]^2 \rangle. \tag{1}$$

The parameter $\sigma$ is termed the rms roughness.

The function $g(L)$ is related to the height–height correlation function [7]

$$C(L) = \sigma_\infty^2 \exp(-(L/\xi)^{2H}) = \sigma_\infty^2 - \frac{1}{2} g(L) \tag{2}$$

yielding

$$g(L) = 2\sigma(L)^2 = 2\sigma_\infty^2 [1 - \exp(-(L/\xi)^{2H})] \tag{3}$$

which saturates when $L \gg \xi$ at $g(L) = 2\sigma_\infty^2$ and varies as $g(L) \sim L^{2H}$ when $L \ll \xi$. The parameters $\xi$ and $H$ are the correlation length and the Hurst dimension respectively.

These calculations require that the histogram of heights over the surface [9] follows a Gaussian distribution [10]; this requirement was fulfilled in our case.

Although the scanning tunnelling microscope (STM) is an ideal instrument for surface roughness analysis, having a dynamical range of structure sensitivity extending over several decades, no discussion of roughness measurements can be complete without a treatment of the effects of image artifacts. There are two common phenomena to take into account for STM: the finite radius of the tip and the slope present in the image.

The effect of tip radius has been discussed by several authors [11, 12] and it is clear that it affects the measured roughness [13]. A suitable criterion to use for assessing the possible influence of the tip sharpness on the reliability of the roughness values obtained is given by Griffith and Grigg [14]. However, for *in situ* UHV measurements, characterization and maintenance of a particular tip geometry is difficult. Thus, it is impossible to define a radius for our tips. However, they are sharp enough for us to resolve atomic steps of the Fe film even down into the steepest depressions, and various measurements with different tips give reproducible roughness results. Therefore we conclude that our results are independent of the actual tip shape and represent the true Fe film roughness.

A proper treatment of the plane fitting is essential, since application to images with dimensions smaller than the correlation length will inevitably lead to erroneous results. We plane fitted STM images ranging in scan size from 50 to 500 nm, having dimensions clearly larger than the correlation length in order to avoid errors by removing any macroscopic slope present in the image. This was done by subtracting a least-squares-fitted plane from the image. ‘Flattening’—that is, subtracting the average slope from each scan line—was thought to be inappropriate since it distorts the image.

Afterwards, we divided each of these images successively into 4, 9, 16, 25, 64, 100 and 256 square, non-overlapping tiles of decreasing linear dimension $L$, and computed $\sigma$ for each tile. The mean of $\sigma$ over all tiles with the same dimension $L$ then gives a final value for $\sigma(L)$ for a given $L$ [13]. This procedure ensures also that the smaller images are correctly slope corrected using the average plane found for the large original image. These tile sizes almost exactly cover the whole image, each pixel being used once. The standard deviation of the values of $\sigma$ computed for the tiles can be used to assess the error in this procedure. These error bars fell within the spread of data for successive scans of the surface. We removed images from the data-set which showed gross and obvious defects such as large areas where contaminants are present or resolution is lost. This was the sole criterion for removing data.

Figure 1 shows the relation between $\sigma$ and the tile edge length, $L$, plotted using a log–log scale. Each line in the figure was derived from a single complete scan of the

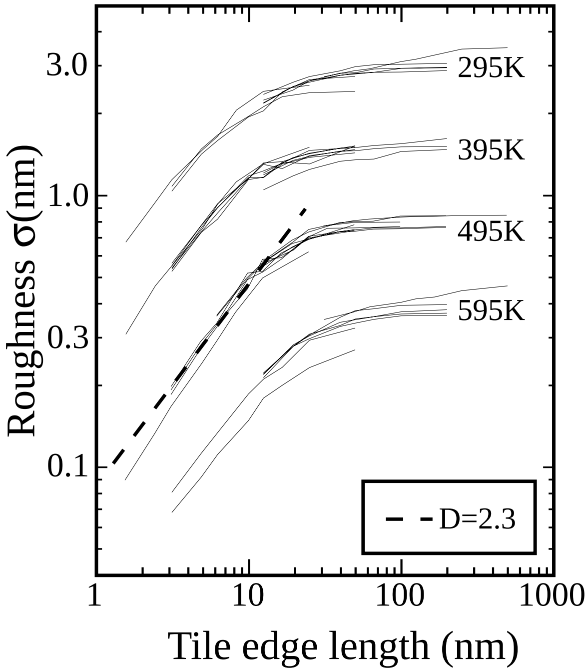

**Figure 1.** The relation between the roughness, $\sigma$ and the tile edge length $L$. The data have been scaled to separate the curves in the $y$-direction; the numerical values of $\sigma$ at 200 nm can be read off from table 1. Straight-line segments are drawn between data points.

**Table 1.** The fractal dimension $(D)$, correlation length, average island size and rms roughness averaged over a single 200 nm image summarized. The standard deviation of the island sizes was approximately 15% in all cases.

| Growth temperature (K) | $D \pm 0.1$ | $\xi \pm 2$ (nm) | Mean island size (nm) | $\sigma_\infty$ (nm) |
|---|---|---|---|---|
| 295 | 2.4 | 15 | 7 | 0.52 |
| 395 | 2.3 | 12 | 9 | 0.42 |
| 495 | 2.1 | 19 | 15 | 0.58 |
| 595 | 2.3 | 29 | 31 | 0.28 |

surface. The small spread of the lines indicates the quality and reproducibility of our data and the absence of tip shape artifacts in the estimation of the roughness values. For all deposition temperatures, $\sigma(L)$ first increases with $L$ and then saturates for larger $L$. The initial slope is related to the Hurst dimension $H$, the location of the intermediate region gives the correlation length $\xi$ and the curves saturate at $\sigma_\infty$.

The behaviour for $L \gg \xi$ will be discussed first. When the tile edge length, $L$, is much greater than the size of typical features, increasing $L$ still further does not bring higher features into a typical tile. Table 1 gives the values of $\sigma_\infty$ averaged over several *complete* 200 nm images. This number is the only meaningful estimate of the rms surface roughness, since, for smaller images, $\sigma$ becomes length dependent, making a comparison of different images impossible. The observed reduction of $\sigma_\infty$ with increasing deposition temperature of the Fe films is associated with the large flat islands which appear at the highest temperature [8].

When $L$ is much smaller than $\xi$, $H$ can be determined. It is related to the fractal dimension by $D = 3 - H$. Table 1 gives values of $D$ found by least-squares fitting of data with $L < 8$ nm. Obviously, the Fe films show values of $H$ close to 2/3 ($D \approx 2.3$), independently of the deposition temperature.

The values of $\xi$ were determined for each deposition temperature by least-squares fitting using equation (3). In order to reduce the number of free parameters, $H$ was fixed at 0.72 (the average over all four temperatures) and $\sigma_\infty$ was fixed at the value given in table 1. The values of $\xi$ clearly indicate an increase in island size with growth temperature [8]. Between 295 and 395 K, the islands not only become visibly larger and squarer, but the difference in heights between islands is lower. This results in a both a smaller $\sigma_\infty$ and smaller $\xi$, although the average island size is marginally larger. Average island diameters along the major axes are also given in table 1; these were obtained by measuring the distance between the trenches on opposite sides of well-defined islands. For the higher temperatures, $\xi$ is close to the average size, but twice as large as 295 K, indicating the stronger variation of island heights for lower deposition temperatures. For none of the growth temperatures could we observe growth pyramids with [012] facets as described by Thürmer *et al* [15]. However, these can perhaps only be observed in Fe films much thicker than the ones investigated here.

The statistical values of the dependence of the surface roughness of epitaxial Fe layers on MgO(001) on the deposition temperature obtained here provide valuable information for calculations of electric properties such as the electron surface scattering [16]. This is a prerequisite for the understanding of the transport properties of single Fe films [17] and superlattices containing Fe [18].

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