Available online at www.sciencedirect.com
SCIENCE DIRECT®
Surface Science 594 (2005) 212–220
SURFACE SCIENCE
www.elsevier.com/locate/susc

# Investigation of the structure of ultra-thin films of Fe on Cu(1 1 1) using medium-energy ion scattering

M.D. Cropper [a,*], T.C.Q. Noakes [b], M.T. Butterfield [a,1], P. Bailey [b]

[a] *Department of Physics, Loughborough University, Loughborough LE11 3TU, UK*
[b] *CLRC Daresbury Laboratory, Daresbury, Warrington, Cheshire WA4 4AD, UK*

Received 13 June 2005; accepted for publication 11 July 2005
Available online 11 August 2005

**Abstract**

The structure of a 12 ML ultra-thin film of Fe on Cu(1 1 1) has been investigated using medium-energy ion scattering. The as-deposited film was found to be poorly ordered with a mean square static displacement of 0.23 Å However, the order was improved by post-deposition annealing using temperatures up to 250 °C, which reduced the mean square static displacement to 0.15 Å. The structure of the as-deposited film was consistent with a poorly ordered Kurjumov–Sachs coincidence—$(1\,1\,1)_{fcc}\|(1\,1\,0)_{bcc}$, $[\bar{1}\,1\,0]_{fcc}\|[\bar{1}\,1\,1]_{bcc}$, $[1\,1\,\bar{2}]_{fcc}\|[\bar{1}\,1\,\bar{2}]_{bcc}$—as reported by other workers, but with some evidence of coexistence of other orientations. Upon annealing the more-ordered film structure was dominated by the Greninger–Troiano orientation—$(1\,1\,1)_{fcc} \sim 1°$ from $(1\,1\,0)_{bcc}$, $\langle 1\,1\,2\rangle_{fcc} \sim 2°$ from $[1\,\bar{1}\,0]_{bcc}$—with coexistence of both Kurjumov–Sachs and Nishiyama–Wassermann—$(1\,1\,1)_{fcc}\|(1\,1\,0)_{bcc}$, $[\bar{1}\,0\,1]_{fcc}\|[0\,0\,1]_{bcc}$, $[\bar{1}\,2\,\bar{1}]_{fcc}\|[\bar{1}\,1\,0]_{bcc}$—coincidences.


*Keywords:* Iron; Fe; Copper; Cu(1 1 1); Epitaxy; Growth; Orientational relationship; Kurjumav–Sachs; Greninger–Troiano; Nishiyama–Wassermann; Medium-energy ion scattering (MEIS); Disorder

## 1. Introduction

There is a large international activity in metal-on-metal epitaxy, motivated in part by the desire to produce metastable phases of magnetic transition metals. One element that can be produced in artificial structures with many interesting properties is iron. Iron is bcc at room temperature but the use of closely matched substrates has enabled the production of (fcc) γ-Fe, with a rich variety

* Corresponding author. Tel.: +44 1509 223308; fax: +44 1509 223986.
*E-mail address:* m.d.cropper@lboro.ac.uk (M.D. Cropper).
[1] Present Address: Materials Science & Technology Division, Chemistry & Materials Science, Lawrence Livermore National Laboratory, P.O. Box 808, L-367, Livermore, CA 94550, USA.

0039-6028/$ - see front matter 
doi:10.1016/j.susc.2005.07.025

of magnetic properties, depending mainly upon the lattice spacing. The growth of γ-Fe has been studied on the (100) [1], (110) [2] and (111) [3–13] faces of Cu under a variety of conditions. Whilst the growth γ-Fe of on the (100) surface of Cu is well behaved, the growth on the closer packed (111) is much more complex.

The interest in Fe on Cu(111) has motivated several investigations of its structure. It has been studied by low energy electron diffraction (LEED) [3–6], angle-scanned photoelectron diffraction [5], energy-scanned photoelectron diffraction [7], scanning tunnelling microscopy (STM) [8–11], surface EXAFS [12] and normal incidence X-ray standing wave [13]. It is widely reported that Fe grows in a pseudomorphic fcc structure for the first few monolayer equivalents. Some LEED/AES investigations reported layer-by-layer growth [3,4], but angle-scanned photoelectron diffraction [5] and STM [10] measurements have shown that the Fe grows in 3-D islands and that the initial islands are mostly of bilayer height.

With increasing thickness, the Fe film relaxes to bcc, as determined by LEED [3], angle-scanned photoelectron diffraction [5], energy-scanned photoelectron diffraction [7] and surface EXAFS [12]. It is generally accepted that the bcc structure registers onto the fcc substrate with the Kurjumov–Sachs (KS) orientational relationship. This has the bcc(110) direction of the film normal to the surface and closely packed rows of atoms of both structures aligned. It is now thought that the transition begins between 2 and 4 ML, with a true bcc structure being present by about 5–8 ML. The angle-scanned photoelectron diffraction [5] and surface EXAFS [12] measurements indicated a transition region where neither fcc nor bcc was a good description, and that it was possible that domains of both were coexisting. The energy-scanned photoelectron diffraction [7] measurements, however, reported an abrupt transformation with the entire film converting to bcc. In contrast, STM images [10] show bright needle like areas that are considered to be needle like domains of bcc Fe sitting on fcc Fe.

The growth of a bcc(110) structure on an fcc surface plane is necessarily imperfect due to the difference in internal angle in the unit mesh. In the case of fcc(111) the internal angle is 120° whereas for bcc(110) it is 109.5°. This mismatch may lead to strain in the mesh resulting in a modification of the mesh shape and/or size. In particular, if in the KS orientation the closely packed bcc[$\bar{1}$11] and fcc[$\bar{1}$10] are aligned, then the open directions bcc[$\bar{1}$10] and fcc[$\bar{2}$11] must be out of alignment by, in principle, 5.3°. However, it is known that in the case of Fe on Cu(100) [1] small misalignments occur in the overlayer. To determine precise alignments in a system like Fe on Cu(1111) requires a method that is very precise in its measurement of angles. The imperfection of the matching of the film to the substrate is manifest in the LEED patterns reported, which have one-dimensional broadening of the spots indicating that there is a spread of alignments around the KS orientation.

Medium-energy ion scattering (MEIS) is a real space technique that allows the determination of surface and near-surface structures [14,15]. Surface crystallography may be determined by analysis of (incident) shadowing and (outgoing) blocking phenomena of elastically scattered ions, and by analysing the angular locations of the outgoing blocking dips at fixed incident directions. In addition to the elastic energy loss, inelastic processes reduce the energy of the ions by an amount proportional to path length through the surface region, enabling the depth of the scattering event to be determined. Thus MEIS is a structural technique with a depth resolution close to that of a single atomic layer thickness.

Despite the interest in the Fe on Cu(111) system, there have been few if any quantitative investigations into order and the influence of annealing on the structure. We have applied the method of MEIS to the study of Fe ultra-thin films deposited on Cu(111). The focus of the work has been on the degree of order in the films and the quantification of the orientational relationship between the bcc Fe overlayer and the fcc Cu substrate.

## 2. Experimental

The MEIS measurements were made using CLRC central facilities [16] based at Daresbury