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Image processing for grazing incidence fast atom diffraction

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ABSTRACT

Grazing incidence fast atom diffraction (GIFAD, or FAD) has developed as a surface sensitive technique. Compared with thermal energies helium diffraction (TEAS or HAS), GIFAD is less sensitive to thermal decoherence but also more demanding in terms of surface coherence, the mean distance between defects. Such high quality surfaces can be obtained from freshly cleaved crystals or in a molecular beam epitaxy (MBE) chamber where a GIFAD setup has been installed allowing in situ operation. Based on recent publications by Atkinson et al. (2014) and Debiossac et al. (2014), the paper describes in detail the basic steps needed to measure the relative intensities of the diffraction spots. Care is taken to outline the underlying physical assumptions.

1. Introduction

MBE is the reference technique to produce very high quality crystalline surfaces while GIFAD is sensitive to surface coherence over length scales in the range of 1000 Å [2–4]. Recently, combining both techniques has increased the surface sensitivity of MBE diagnostics while providing surfaces with exceptional quality for in situ fast atom diffraction. GIFAD can be operated easily both in growth condition where almost video rate was demonstrated [1], and in high resolution mode, before or after growth, where its sensitivity poses a challenge to the theoretical description [2]. The present paper focuses on the data analysis and the associated physics. To support the discussion the data presented here are taken from Ref. [2] and [1]correspond to a GaAs surface grown in situ by homo-epitaxy and held at a temperature of 570 °C under an As_4 overpressure during the measurements.

2. GIFAD and MBE

GIFAD has been described in several places (see e.g. [5]) and only a brief sketch is given here in Figs. 1 and 2. Just as HAS, helium atoms are weakly attracted by van der Waals forces and strongly repelled by the surface electronic density. In terms of interaction geometry, as seen on Fig. 2, GIFAD is similar to reflection high energy electron diffraction (RHEED). In a way GIFAD is to HAS what RHEED is to low energy electron diffraction (LEED) as illustrated in Table 1.

An important practical difference is that keV atoms are used which can be detected with high efficiency and that the diffraction cone is kinetically compressed allowing the full pattern to fit onto a position sensitive detector. As a simplification, GIFAD can be seen as a projected technique where only the movement perpendicular to the surface plane is important [6–8]. If the helium beam is well-aligned with this low index direction forming only an angle θ with the surface plane, the energy $E_\perp$ of the movement normal to the surface is given by $E_\perp = E_0 sin^2\theta$ with E_0 the energy of the primary beam. This energy $E_\perp$ can be tuned between few meV up to few eV with only a degree variation as illustrated in Fig. 3. Note that the wavelength $\lambda_\perp$ associated with this slow motion is in the Å range.

3. Data analysis

3.1. Primary beam, Laue circle and incidence plane

We will not consider the nature of the position sensitive detector used to record the diffraction pattern as a 2D image. We assume here that the detector is far from the surface and perpendicular both to the surface plane and to the plane of incidence so that the number of counts in each pixel (x,y) corresponds to an intensity map in momentum space $I(k_x, k_y)$. In the present case, one CCD pixel corresponds to a scattering angle of 0.004 deg. or 7 10^{-5} rad. As with standard crystallography two type of information can be extracted, the surface lattice unit is reflected in the peak spacing while the relative peak intensities depend on the

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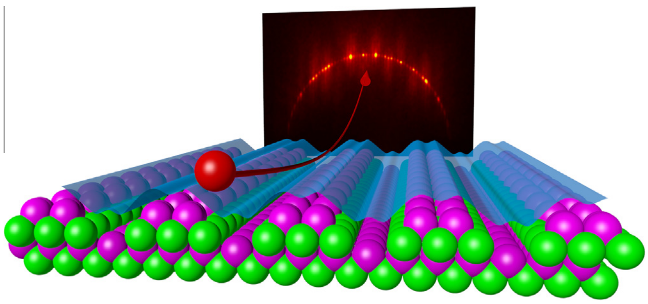

Fig. 1. Schematic view of a GIFAD arrangement [2], the primary beam of helium atoms does not really see individual atoms but are reflected by the periodic electronic density of well-aligned rows of atoms.

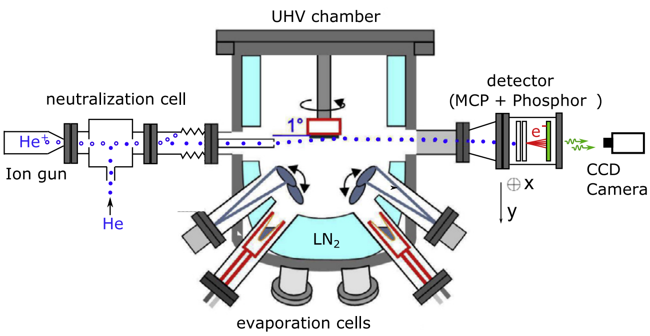

Fig. 2. Schematic view of the MBE chamber [1], with effusion cells evaporating gallium and arsenic onto the GaAs(001) wafer. A He^{+} ions beam is extracted from a commercial ion source and is neutralized before entering the vessel. The atoms scattered by the surface are imaged onto a position sensitive detector.

Table 1
Names of electron and atomic diffraction techniques.

Geometry\proj.	Electrons	He atoms
Normal incidence	LEED	HAS,TEAS
Grazing incidence	RHEED	GIFAD

scattering amplitudes determined here by the shape of the electron density at the surface. The treatment starts by a precise determination of the primary beam parameters; its location x_b, y_b and its width which is measured here by its fwhm $\sigma_b = 3.6$ pixel or 0.25 mrad, symmetric along the x and y directions. This can be achieved before or after the diffraction by removing the target surface or, during diffraction by leaving a small part of the beam flying over the surface without interaction, as can be seen as a tiny spot at the bottom of Fig. 3a–c. In favorable cases such as those depicted in Fig. 3, the Laue circle, defined by energy conservation ($|k_{out}| = |k_{in}|$) is clearly visible by interpolation between the elastic diffraction spots, and thus its center coordinates x_L, y_L and radius R_L are easy to pinpoint. However, this does not specify the scattering plane, defined on the detector by a line linking the primary beam to the specular beam[2,9]. If the direct beam is perfectly aligned with the low index crystal axis of the surface, the specular spot is easy to identify as the symmetry center but the alignment step can be tricky if no precautions have been taken [6,7,9]. Here we assume that the scattering plane is identified as the vertical axis so that the horizontal axis of the image is parallel to the surface plane. The goal is now to extract the intensity along the Laue circle and to assign, as precisely as possible, the intensity of each diffraction spot.

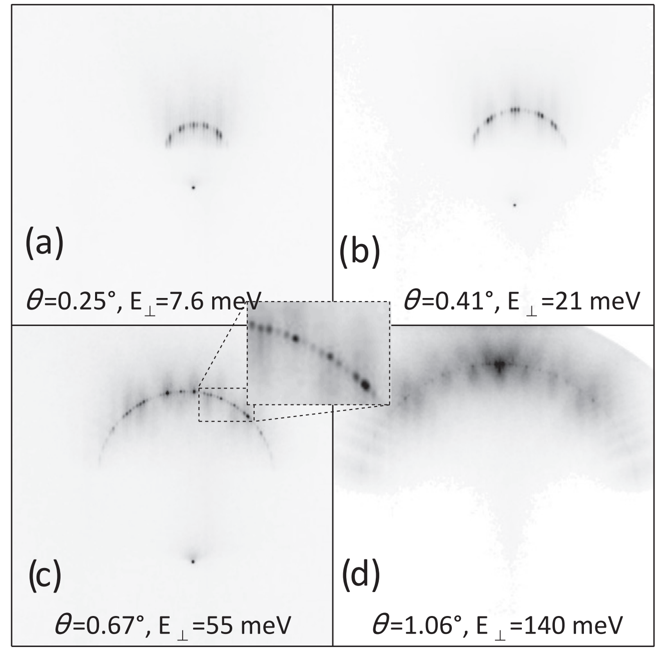

Fig. 3. Four diffraction patterns recorded for a E_0 = 400 eV He primary beam aligned along the [1–10] direction of the GaAs(001) surface held at 570 °C corresponding to the $\beta_2(2\times4)$ reconstruction [2]. The diffractions spots are located on the Laue circle which radius is equal to the angle of incidence θ. From (a) to (d) θ is increased from 0.25–1.06 deg. allowing a factor close to 20 in normal energy $E_\perp = E_0 sin^2\theta$ between the first and fourth image.

3.2. Background subtraction

In Figs. 3 and 6a some intensity is present below and above the Laue circle. Its contribution increases with the angle of incidence, i.e. with the normal energy $E_\perp$ from Fig. 3a–d. This intensity, originating both from inelastic scattering [10], and from surface imperfections [11,12], is very interesting in itself providing information on the surface Debye temperature and on specific phonon properties. However, our concern here is only to derive the (periodic) topological properties of the surface by extracting the elastic diffraction signal, i.e. the intensity associated with the sharp spots sitting exactly on the Laue circle. As can be seen in Fig. 3, the background to be subtracted is far from uniform showing both diffraction features in the horizontal direction and pronounced patches along the vertical direction as well as a quasi-nodal structure along oblique directions [13]. These structures originate from quasi-elastic scattering processes [10] which is closely linked to the elastic scattering [10]. Similar patches are indeed present in diffraction charts when the diffracted intensities on the Laue circles [2,14,15] are plotted as a function of the angle of incidence (see also Fig. 8). The reason is that the diffracted intensity can be written as an expansion in terms of the number of exchanged phonons. Close to the Laue circle, this number should be limited and the inelastic signal should resemble the elastic one in terms of intensity ratio of the various diffraction orders [16]. The fact that this background looks similar to the intensity on the Laue circle is a favorable condition for reasonable corrections. One way to estimate this contribution is to consider it as varying slowly in the vertical direction so that it can be interpolated from its values above and below the Laue circle by a linear interpolation. In practice, the background intensity $I_{back}(x, y)$ at any pixel (x, y) on the Laue circle is estimated as $I_{back}(x, y) = [I(x, y + u) + I(x, y - u)]/2$ where the distance u will be chosen as small as possible but not smaller than the experimental resolution. This is equivalent to a double differentiation. To make this subtraction easy and not too noisy we use the smoothest