Applied Surface Science 288 (2014) 458–465

Contents lists available at ScienceDirect

Applied Surface Science

journal homepage: www.elsevier.com/locate/apsusc

Instrument response of reflection high energy electron diffraction pole figure

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ARTICLE INFO

Article history:
Received 10 April 2013
Received in revised form 5 October 2013
Accepted 10 October 2013
Available online 18 October 2013

Keywords:
Reflection high energy electron diffraction
RHEED pole figure
Instrument response of transmitted electrons
Epitaxial CdTe film
Textured CdTe film

ABSTRACT

Reflection high-energy electron diffraction (RHEED) pole figure technique using the transmission mode has been developed to study the texture evolution of thin films. For quantitative evaluation of thin film texture, including the dispersion of texture, one would require the knowledge of the instrument response function. We report the characterization of instrument response in RHEED pole figure from an epitaxial CdTe(1 0 0) film grown on GaAs(1 0 0) substrate. We found the finite mean free path of electrons in a film contributes to the broadening of the poles. In addition, the image processing step size used in the construction of a pole figure also affects the broadening of constructed poles. We apply the measured instrument response in RHEED pole figure to quantitatively analyze a biaxially textured CdTe(1 1 1) film deposited on a biaxially textured Ge(1 1 1) substrate. Through the deconvolution of the measured dispersions from the poles in the textured CdTe(1 1 1) film by the instrument response function, we obtain the out-of-plane and in-plane dispersions of the biaxially textured CdTe(1 1 1) film. This method is generic and the instrument response should be considered in order to obtain quantitative texture information for other epitaxial and textured nanostructured films through RHEED pole figure measurements.

1. Introduction

Diffraction techniques such as X-ray diffraction and electron diffraction are essential tools to study the crystallography of materials. They are also useful for detecting crystal imperfections, which manifest themselves as distortions in the diffraction profiles [1]. One of the common distortions is a broadening of the diffraction profiles. For a quantitative study of crystal imperfection, one would require to know the distortion, including the broadening, due to inherent instrumental effects called the instrument response function [2]. The nature of the instrument response function had been studied quantitatively in detail and had been reported in the literature for diffraction techniques [3–6]. Any observed X-ray or electron diffraction profile is a convolution of the instrument response function with the intrinsic diffraction profile that reflects the characteristics of a crystal. In order to quantitatively extract the intrinsic properties of the crystal imperfections, one has to de-convolute the observed diffraction profiles by the instrument response function. This strategy has been applied routinely in X-ray diffraction and electron diffraction techniques.

A more sophisticated way to represent crystal imperfections is the pole figure technique. A pole figure is a 2-D graphical representation of the crystal orientation distribution. It is in the form of spherical projections of 3-D orientation distribution of the crystal lattice planes onto a 2-D figure. If the crystals were not perfect, the pole figure would show a distortion of the pole intensity distribution. A pole figure is constructed, using either a point detector or an area detector, by scanning the diffraction intensity profiles over the diffraction space above the sample. A finite scanning step size is normally chosen for this construction. Because of the large diffraction space that the X-ray pole figure needs to cover, the step size usually is chosen to be larger than that used in an individual X-ray rocking curve or in an individual reflection high-energy electron diffraction (RHEED) streak profile. For example, to scan a rocking curve of a film using X-ray point detector, the step size for the detector used is often very small (<0.005°). Since only one diffraction spot is scanned, it takes a reasonable time to complete a rocking curve scan even using a small step size. However, to scan the entire diffraction space using a very small step size to construct the pole figure is not very realistic. For example using 0.005° as the step size and 1 s as the rest time, it would take 360,000 h ($360 \times 90/0.005/0.005 \times 1$ s) to obtain a complete X-ray pole figure, which is not realistic. Therefore, to save the data acquisition time, the step size chosen to construct a pole is usually much larger than 0.005°.

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http://dx.doi.org/10.1016/j.apsusc.2013.10.055

However, using a large step size to acquire intensity profiles and to construct the pole figure would inevitably distort the pole intensity distribution. It becomes an additional contribution to the instrument response function during data acquisition. Its effect needs to be included if a quantitative evaluation of the pole figure is considered. In this work, we use RHEED patterns to construct a RHEED pole figure. Each RHEED pattern is a two dimensional image, which contains the χ direction (or polar angle direction from the surface normal) intensity distribution for a particular ϕ angle (azimuthal angle parallel to the surface). One has to select a step size for processing the intensity profile from many two dimensional intensity patterns to construct this χ scan in a pole figure. We give a quantitative analysis of the effect of the step size on the RHEED pole figure construction. To construct a pole figure we used RHEED transmission mode from surfaces that possess nanoscale roughness. We present the RHEED pole figure construction of a CdTe(1 0 0) film epitaxially grown on single crystal GaAs(1 0 0) surface as an example of how to obtain the instrument response function. We then applied the measured instrument response function and deconvoluted it from the total instrument response obtained from textured CdTe(1 1 1) film grown on biaxial Ge(1 1 1) film to obtain the texture dispersion of CdTe(1 1 1) film grown on Ge(1 1 1). Through the experiments we identify two new factors that contribute to the transmission RHEED pole broadening, the finite inelastic mean free path of 15 keV electrons and the processing step size in the construction of RHEED pole figure.

2. Instrument response of a pole figure: general discussion

For X-ray diffraction, if the crystal sample is perfect and infinitely large, one expects a broadening purely due to the instrument response. Examples of instrumental effects in X-ray diffraction include the beam divergence, energy spread, and beam width [6,7]. This intrinsic instrument response function is denoted by T_i. The broadening of the diffraction profile due to instrument response translates into the broadening of the intensity concentrations in the X-ray pole figure. In order to construct the pole figure, as we discussed above, one requires scanning the intensity over the whole diffraction space. In doing so, one inevitably needs to choose a reasonably large step size (window) to record the intensity for the construction of a pole figure. The value of this step size would contribute to the broadening of the poles and would become a part of the effective instrument response of the pole figure constructed. The overall instrumental broadening T_I for the pole, therefore, is the convolution of the T_i with the broadening due to the finite step size T_s: $T_I = T_i \times T_s$. The step size broadening, in principle, could be minimized by choosing a very small step size. A schematic illustrating the instrumental broadening in an X-ray pole figure is shown in Fig. 1(a).

For X-ray diffraction, if a sample consists of finite size crystals (e.g., less than 100 nm) with the same orientation, then the diffraction profile due to this finite crystal size effect will have an additional broadening T_f on top of the instrumental broadening T_I. The total diffraction profile observed will be $T_I \times T_f = T_i \times T_s \times T_f$. The corresponding pole figure is shown schematically in Fig. 1(b). For crystals having other imperfections such as the out-of-plane and in-plane dispersions, the pole intensity concentrations will be further broadened as shown in Fig. 1(c).

Similar to X-ray diffraction, RHEED profile also has an instrument response function T_i due to instrumental effects including electron beam divergence, energy spread, and beam diameter [2,3]. For our purpose, an area detector (phosphorous screen) is used. Unlike the X-ray photon, the electron has a much shorter inelastic mean free path (IMFP) [8]. The electron typically can only penetrate and transmit through finite size of the crystals, which are much smaller than that in X-ray diffraction. The electron finite size transmission from crystals would give raise to a broadening of the diffraction profile T_{ft}. Note that in X-ray diffraction, the finite size broadening T_f is due to the effect of real finite crystal size. In RHEED, T_{ft} is due to the IMFP, which is part of the instrumental effect.

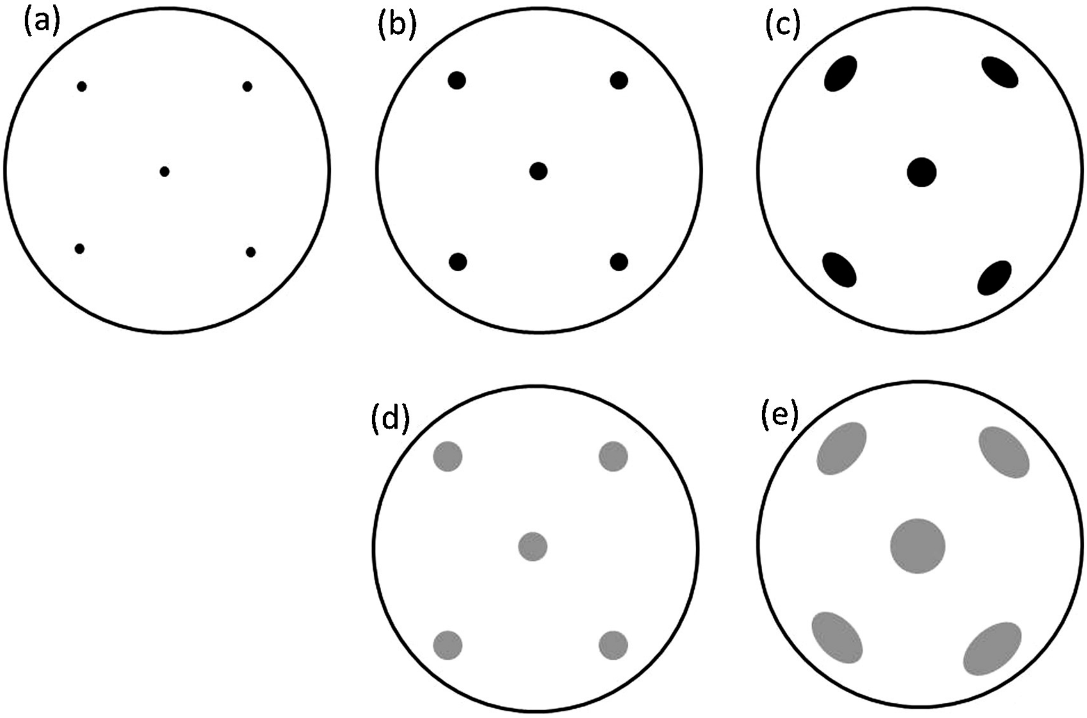

Fig. 1. (a)–(c) are schematics showing pole intensity distributions in X-ray pole figures due to instrumental broadening, finite size crystal broadening, and biaxial texture dispersion broadening, respectively. (d) and (e) are schematics showing pole intensity distributions in RHEED pole figures due to a combined instrumental and finite crystal size broadening as a result of finite inelastic mean free path and biaxial texture dispersion broadening, respectively.