Dynamical x-ray reflection at terraces in epitaxial layers

Shih-Lin Chang

Max-Planck-Institut für Festkörperforschung Heisenbergstr. 1, 7000 Stuttgart 80 Federal Republic of Germany

(Received 29 June 1981; accepted for publication 13 August 1981)

Terrace formation in semiconductor epitaxial layers has been postulated to cause lattice bending, which ought to be observable by x-ray diffraction. Consideration of dynamical effects of x-ray reflection, both at the terraces and from a distorted crystal lattice, shows that diffraction effects by far outweigh the effects of lattice bending. For a given liquid phase epitaxial GaAs layer on a GaAs substrate, the lattice bending is estimated to be less than $10^{-3}$ rad.

PACS numbers: 61.10.Fr, 68.55. + b

Epitaxial layers of semiconductor materials, as grown from chemical vapor deposition, liquid phase (LPE), vapor phase (VPE), and molecular beam epitaxy, usually exhibit morphological unevenness, such as terraces, hillocks, and pyramids. Terraces have recently received particular attention concerning formation mechanisms and substrate-orientation dependence. A theoretical model, proposed by Rode, is intended to account for the formation of terraces by means of atomic step bunching due to elastic deformation of the crystal lattice. Observations on the surface morphology and the growth rate of epitaxial layer as a function of the angle of misorientation in the substrate seem to support the theory indirectly.

A direct detection of lattice distortion, caused by step bunching, of [001] LPE GaAs layers on GaAs substrates has been attempted recently by Sullivan and Hagen with double-crystal x-ray topography. In their experiments, topographs of [224] reflections were taken at the angular positions $\theta_-$ and $\theta_+$ [Fig. 1(b)], at which half-maximum intensities were obtained. Topographs with definite contrast were seen. They are reproduced here in Fig. 2. The terraces are approximately 1 $\mu$m in height and 40 $\mu$m in width for the treads and risers, respectively. Image contrast reverses when the Bragg angle $\theta$ changes from $\theta_-$ to $\theta_+$ as well as when the crystal is rotated by 180°, i.e., from [224] to [224]. A lattice distortion due to bending has therefore been suspected. Dynamical diffraction effects from the zig-zag surface could, however, mask the whole topographic images. This phenomenon has frequently misguided the interpretation of topographs. In this letter, I consider the effects of both terraced surface geometry and presumed lattice bending on dynamical Bragg reflection. I eliminate the ambiguity on interpreting the double-crystal topographs and conclude that the boundary effect of dynamical diffraction plays a major role in the topographic image contrast, while lattice bending adds only a second-order effect. In the experiment of Sullivan and Hagen, the lattice bending is not greater than $10^{-3}$ rad.

The geometry representing an asymmetric Bragg reflection in reciprocal lattice space is shown in Fig. 1(a). By considering the plane-wave dynamical theory of x-ray diffraction, the corresponding wavefield-amplitude ratio $|E_H/E_0|^2$ of the reflected beam $H$ and the incident beam $O$ are plotted in Fig. 1(b). $A$ and $B$ are the components of the terrace. $LaE$ is the incident wavefront. $La$ and $Lo$ are the Laue and Lorentz points, respectively, $d_H = OH$ is the reciprocal lattice vector of the reflection $H$. The [224] reflections of the Si monochromator crystal and of the GaAs sample were almost completely linearly polarized in the direction normal to the plane of incidence. In reflection, the incident waves can excite the "solution" dispersion surface, which is indicated by the broad solid curve in Fig. 1(a), rather than the dashed hyperbolic one which holds for the transmission case. The region in between the hyperbolic branches is known as the total reflection range, which has values of $|E_H/E_0|^2$ close to unity.

For the crystal at $\theta = \theta_-$, the corresponding wavefront lies in the vicinity of point $C$. With respect to the crystal surface $A$ and $B$, the incident waves excite two different parts of the reflection $H$, the corresponding wavefield-amplitude ratio $|E_H/E_0|^2$ of the reflected beam $H$ and the incident beam $O$ are plotted in Fig. 1(b). $A$ and $B$ are the components of the terrace.
A small lattice distortion, for example, lattice bending, would shift the dispersion surface parallel to LaE in direction either towards or away from the Laue point. The former situation with a lattice bending of 10 in. (5 x 10^{-5} rad) is schematically shown in Fig. 3, where δg is the distortion introduced by the bending. L_{\theta} and d_{\mu} are the new Lorentz point and reciprocal lattice vector. Because the new dispersion surface (dashed) in the total reflection region is excited by the incident beam with respect to both A and B, the reflected intensity from A is about equal to that from B at ϑ = ϑ_+, while the intensity at ϑ_- is rather weak. The experimental images of Fig. 2, however, do not possess this characteristic. It is, therefore, reasonable to say that the lattice bending in this particular sample must be less than 10^{-5} rad. This small amount of bending modifies the image contrast only in second order.

In conclusion, we have, on one hand, qualitatively demonstrated that by considering the boundary effect on the dynamical reflection one can distinguish the topographic image contrast of dynamical diffraction from that of lattice distortion. On the other hand, for the epitaxial materials having clear topographic images as shown in Fig. 2, the lattice bending, if it exists at all, should be less than 10^{-5} rad. For detailed quantitative analyses, the dynamical theory of Penning and Polder\(^{11}\) must be applied for in calculating the reflected intensity in relation to lattice distortion. This calculation is now under way; results will be reported later.

The author is indebted to Professor H. -J. Queisser for raising this problem and for his encouragement and helpful discussion. Particular acknowledgments are gratefully extended to Dr. P. A. Sullivan and Dr. W. Hagen for providing their informative and carefully recorded topographs.

---

6. P. A. Sullivan and W. Hagen analyzed their data with the kinematical theory and realized the alternative of a dynamical effect (private communication).