Epitaxial Growth
Studied by Surface X-Ray Diffraction

J.E. Macdonald¹, C. Norris², E. Vlieg³, A. Denier van der Gon³, and J.F. van der Veen³

¹University College, Cardiff CF11XL, United Kingdom
²University of Leicester, Leicester LE17RH, United Kingdom
³FOM Institute for Atomic and Molecular Physics,
Kruislaan 407, NL-1098 SJ Amsterdam, The Netherlands

Epitaxial growth is intimately related to the presence of steps, islands and other forms of surface irregularity. The characterisation of atomic disorder at a surface is therefore central to our understanding of the nature and kinetics of adsorption and, ultimately, to the successful growth of semiconductor structures by molecular beam epitaxy. Surface sensitive diffraction techniques can provide important statistical information about disorder over a wide spatial region. Electron diffraction: LEED and RHEED [1,2] has been used for this but the interpretation is inevitably confused by consideration of the role of multiple scattering. X-ray diffraction, on the other hand, may be interpreted within the kinematical approximation and, with the development of intense synchrotron radiation sources, is finding increasing application in the field of surface crystallography.

Information about surface morphology may be obtained from the wavevector dependence of X-ray reflectivity [3] and crystal truncation rods (CTR's), that is, the Bragg tails arising from the termination of the infinite lattice [4,5]. We report measurements of CTR profiles and reflectivity from a reconstructed Ge(001)2×1 surface using a new surface X-ray diffraction apparatus which allows for the first time in-situ X-ray scattering measurements to be made of a growing surface.

The measurements were made on the wiggler beam line of the Synchrotron Radiation Source at Daresbury Laboratory. Radiation of wavelength 1.58 Å was selected by a channel cut Si(111) monochromator and was unfocussed. The Ge sample was cut and polished to 0.05° of the (001) plane. It was mounted inside a UHV chamber [6] that incorporated Knudsen cells shielded by a cryo-panel, RHEED and sample transfer. A Be window allowed 200° in-plane and 20° out-of-plane access to the sample. The sample holder was coupled to a 5-circle diffractometer via a bellows and a rotary seal. The Ge surface was cleaned by argon sputtering and thermal annealing. Repeated cleaning cycles resulted in a larger (2×1) reconstructed domain size as indicated by transverse scans of the (3/2,0) fractional order peak.

A series of transverse scans were made through the (1,0,l) CTR centred on the Bragg peak which occurs at l = 0.25. This peak corresponds to the (111) reciprocal lattice point in conventional bulk notation. The relation between the surface and bulk notations and the scan directions is illustrated in fig. 1.
The scans are characterised by a sharp peak superposed on a diffuse feature, their relative magnitude being strongly dependent on \( l \) (Fig. 2.). The occurrence of both sharp and diffuse components in CTR scans has been predicted theoretically [4]. The sharp peak results from the long range order between columns of atoms whereas the diffuse component reflects the correlation length for atoms of the same height along the surface. Although both components have been identified with electron diffraction [1,2] previous X-ray studies have only observed the sharp peak.

In this preliminary analysis, we have determined the relative intensity of each component by first fitting the background-subtracted and normalised (to the incident intensity) diffuse feature to a Lorentzian of the form:

\[
\frac{q_{\perp}^2}{I_f^2} = \frac{W_d}{\pi (W_d/2)^2 + q_{//}^2},
\]

where \( I_f \) is the integrated intensity and \( W_d \) the FWHM of the diffuse peak, \( q_{//} \) is the scanned wavevector transverse to the CTR and \( q_{\perp} = (0.25-l)b_3 \) is the wavevector along the CTR, \( b_3 \) being the reciprocal lattice vector perpendicular to the surface. The \( q_{//}^2/f^2 \) term normalises the scattering to that predicted for a sharp interface and to the atomic scattering factor \( f \) for Ge. The integrated intensity \( I_s \) for the sharp peak is summed numerically.