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X-ray scattering from a vicinal Ge(001) surface

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Abstract. High-resolution x-ray diffraction measurements have been made on a Ge(001) surface that had been misoriented by 1.3°. It is shown that the atomic steps formed on the surface are mainly bilayer in height and that the surface reconstructions have domain sizes that are limited by the terrace length between the steps, with both (2 × 1) and (1 × 2) domains present.

It is widely accepted that the Ge(001) and Si(001) surfaces are structurally similar. Both are built up from the same dimer unit oriented along the [110] or [1$\bar{1}$0] axis. Low-energy electron diffraction (LEED) studies of surfaces with mis-cuts in excess of 3° towards the [110] axis have shown the presence of double-layer steps (Olshanetsky *et al* 1977). For Si(001), single-domain (2 × 1) reconstruction results have been consistent with dimer bonds oriented parallel to the step edges (Kaplan 1980). Similar results have been found for Si(001) using TEM (Nakayama *et al* 1987) and STM (Wierenga *et al* 1987). We present here a high-resolution x-ray study of a vicinal Ge(001) surface, which confirms bilayer steps but also shows two reconstructed domains. For non-vicinal (001) surfaces and surfaces oriented towards the [100] axis, single-layer steps have been found. An explanation of this tendency in silicon has been given by Chadi (1987), using a semi-empirical tight-binding calculation. Gadiyak *et al* (1985)—for Ge—and Aspnes and Ihm (1986) agreed with the basic conclusions of Chadi although the precise structure of the steps considered was different.

The measurements were carried out using radiation of 1.38 Å on the wiggler beamline of the SRS at the Daresbury Laboratory. A polished Ge(001) sample was mounted inside a UHV chamber (Vlieg *et al* 1987) coupled to a large five-circle diffractometer. The mis-cut was found by measurement to be 1.34 ± 0.02° towards the bulk [110] axis by reflection of a laser from the surface. After repeated cleaning cycles a sharp RHEED pattern was obtained with both (2× 1) and (1 × 2) superlattice reflections.

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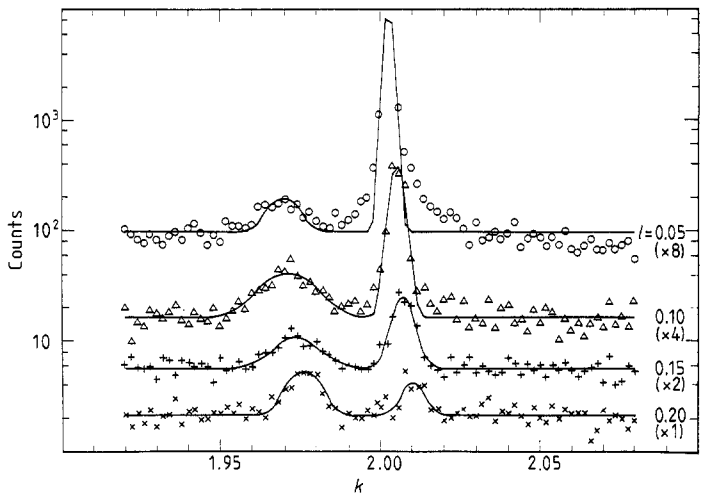

Figure 1. k-scans of the (0 2 l) rod for different l-values.

Table 1.

Reflection			Scan	d (Å)
1.5	0	0.05	k	116.0 ± 10.6
1.5	0	0.05	h	531 ± 120
0	1.5	0.05	k	105.3 ± 16.0
0	1.5	0.05	h	1415 ± 380

Figure 1 shows k-scans at different l-values for the (02l) rod (bulk (220) reflection) plotted on a log scale. With increasing l there is a rapid reduction of the integrated intensity, as is expected from the termination of the surface, and a satellite peak develops due to the long-range correlation of the steps (see Henzler 1970, Ellis and Schwoebel 1968). The separation of the satellite from the main peak in reciprocal space is given by

$$\Delta Q = 2\pi/t$$

where t is the width of the terrace. Referring to the figure gives $t = 118.0 \pm 8.6$ Å for the terrace width. Since the angle of the mis-cut is 1.34 ± 0.02°, we obtain the mean step height to be 2.76 ± 0.25 Å. This compares well with 2.829 Å, the value expected for a double-layer step.

The x-ray scattering pattern revealed the presence of both (1.50l) and (01.5l) rods corresponding to (2 × 1) and (1 × 2) domains. The integrated intensities of both reflections indicated that the ratio of (2 × 1) to (1 × 2) in area was 1.8:1.

Profile measurements of the fractional-order reflections were made for $l = 0.05$ by scanning parallel to h and k. The curves were fitted using a Gaussian, the FWHM corresponding to $5.9/d$, where d is the domain size in real space. We find, after allowing for the instrumental resolution the values given in table 1.

If the domains extended over the whole of the terrace, we would in the present case expect only (2 × 1) domains to be present. However, our results indicate that although the steps limit the size of the reconstructed domain, they do not restrain its orientation.

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