Chapter 5

Structural Defects in GaAs

This chapter deals with the topographic analysis of irradiated GaAs samples. Here, the analysis is based primarily on reflection techniques. As before, the technique of differential topography has been adopted to construct a depthwise image of lattice distortion. In contrast to Si crystals, these samples clearly show an out-of-plane expansion of the irradiated lattice. In samples irradiated to a fluence of $10^{13}$ ions/cm$^2$, such an expansion has been observed also as surface steps measuring $\sim 200$ Å on the stylus.

TRIM Profiles

The TRIM profiles of electronic energy loss (ionization) and ion range distributions are shown in Figs.5.1(a) and (b) respectively. Electronic energy loss at the surface is $\sim 19$ MeV/µm which is about 1.5 times larger than in Si ($\sim 12.5$ MeV/µm, see Fig.4.12 a). Also, it falls faster in this case, i.e. its downward gradient is much larger. The vacancy profile which represents damage due to elastic collisions has its maximum $\sim 18$ µm below the surface. Around its maximum, the number of vacancies produced by a single ion is $\sim 20000/\mu$m which is twice as large as that in Si. Hence the total damage in the implanted sheet is at least double in this case.

5.1 Topographic Analysis

A 220 symmetric transmission scan recorded using Cu K$_\alpha$ radiation is shown in Fig.5.2(a). The masked stripes and the boundary of the irradiated disc have black-white contrast indicating lateral expansion of the irradiated region. In GaAs ($t = 500$ µm) the normal absorption factor $\mu t = 20$ for Cu K$_\alpha$ radiation. Thus, the image of the strain field in this topograph results from dynamically transmitted rays (travelling parallel to the crystal planes) of extremely high angular sensitivity. The white features distributed uniformly over the topograph are the dynamical images of extended defects lying in bulk. Another important observation is the structure of
Figure 5.1: TRIM profiles of 200 MEV Ag$^{14+}$ irradiated GaAs samples – (a) Ionization and vacancy profiles and (b) ion range and vacancy profiles.
the edges of horizontal stripes. In the microscopic enlargement (Fig. 5.2 b), isolated defects are clearly seen. While such defects were absent in 100 MeV Ti$^7^+$ as well as 200 KeV Ar$^+$ irradiated samples, they are also observed at an Ag$^{14^+}$ irradiated Si samples (see Fig. 4.13).

Mo K$_\alpha$ radiation too produces the topographic features with dynamical contrast, its absorption factor in GaAs being 17.5 (see Table-3.2). However, since a dynamical image has a much inferior resolution compared to a direct image, the remaining analysis has been performed in reflection geometry. The analysis has been divided in three parts - the depth analysis of the damaged buried layers, mapping of the distortion interface and investigation of expansion in the irradiated lattice.

5.1.1 Depth Analysis

A novel technique of depth analysis has been discussed in chapter-4. It involves recording a stationary topograph with a narrow (< 10$\mu$m) slit. The distorted lattice produces a diffracted beam in addition to the one diffracted from the surface, the depth of the distorted sheet being inferred from the relative separation of the two beams. The same technique has been applied here as well. A 004 stationary topograph recorded with a 10 $\mu$m collimating slit is shown in Fig. 5.3(a). It is in fact a set of three lines - a continuous line diffracted from the surface and two other lines diffracted from the distorted regions which are discontinuous at the sites of unirradiated stripes. A further enlargement of this topograph is shown in Fig. 5.3(b), and for clarity, the contrast is redrawn schematically in Fig. 5.3(c). The depths of the corresponding
Figure 5.3: (a) 004 stationary topograph (Cu $K_{\alpha}$ radiation), (b) its further enlargement and (c) a schematic representation of contrast.

distorted sheets calculated from separations $S_1$ and $S_2$ (see Fig.5.3 c) are $8 \pm 1 \mu m$ and $18 \pm 1 \mu m$ respectively. Comparing these with TRIM profiles it is obvious that the latter corresponds to the implanted sheet. The other line corresponds to a region close to surface and much above the implanted sheet. This shows that a significant lattice damage also occurs in the electronic loss dominated near-surface region. However, electronic excitations are maximum at the surface and decrease downward whereas the region diffracting additional intensity lies $8 \mu m$ below surface. This can be explained by assuming that the irradiated region undergoes only an overall lattice expansion\(^1\) without losing lattice perfection (i.e it does not become Mosaic). In later sections we present its experimental evidence. On the basis of this the origin of two (discontinuous) lines can be understood as follows—

Due to a negative downward gradient in the deposited energy density (electronic energy loss), the damage and hence the lattice parameter also vary along depth. In topography, only the regions of large strain gradient - where lattice spacing changes rapidly - appear with a contrast in the topograph. On the basis of energy loss profiles (see Fig.5.1), the contrast of Fig.5.3 can be interpreted in terms of a depthwise variation of lattice constant as shown schematically in Fig.5.4. At the surface, the lattice parameter increases due to large electronic energy loss ($\sim 19 \text{ MeV}/\mu \text{m}$). But at a depth of $8 \mu m$, deposited energy density falls below $12 \text{ MeV}/\mu \text{m}$. It is possible that at this point the deposited energy density becomes ineffective in

\(^1\)The lattices of Si and GaAs are known to expand with the introduction of defects.
Figure 5.4: A schematic diagram showing depthwise increase of lattice parameter in the irradiated region. If expansion is assumed proportional to damage, it also represents the damage profile.

terms of actual damage to the lattice. Then a sharp variation of the lattice parameter will occur in this region. As shown in Fig.5.4, the lattice parameter again passes through a maximum close to the implanted sheet due to lattice damage through elastic collisions. Appearance of a diffracted beam from a depth of 8 $\mu$m shows the sensitivity of GaAs to electronic energy loss, threshold being 12 MeV/$\mu$m. No such threshold has been encountered in Si samples. As a result, the actual damage profile in GaAs crystals deviates from the corresponding TRIM profile (see Fig.5.1) where it is assumed that the energy deposited in electronic excitations dissipates in solids without any damage to the lattice.

5.1.2 Distortion Interface

A 004 scan recorded with Cu K$_\alpha$ radiation is shown in Fig.5.5(a). The irradiated zones have dark contrast due to buried distorted sheets. Details of the contrast pattern around unirradiated stripes can be seen in its microscopic enlargement (Fig.5.5 b). Here again, the widths $w_v$ and $w_h$ respectively of the contrast-free vertical and horizontal stripes separating two adjacent dark zones are much wider than the width of the masking grid strips. After correcting for the geometrical contraction, $w_v$ and $w_h$ measured 75±4 $\mu$m and 125±4 $\mu$m respectively. Thus, the dimensional anomaly occurs in these samples as well. The reason for a large difference between the widths $w_v$ and $w_h$ is not immediately clear. But upon successive etches $w_v$ decreases and
close to implanted sheet it equals $w_h$. Hence the initially larger width of vertical stripes is possibly due to a bending of the distorted sheets at the edges. At the edges of the horizontal stripes, the diffraction vector is not sensitive to such bending.

The dark lines within the vertical stripes, with a relative separation $(w_s)$ of $48 \pm 3 \, \mu m$, represent distortion interfaces at the surface. Unlike Si where the contrast covers the entire stripe, here it is sharply defined only at distortion interfaces.

Microscopic enlargements of similar topographs recorded after etching through 3, 7, 11 and 15 $\mu m$ are shown in Figs.5.6(a), (b), (c) and (d) respectively. Table 5.1 shows how the widths $w_s$, $w_v$ and $w_h$ change with etching.

<table>
<thead>
<tr>
<th>Etch ($\mu m$)</th>
<th>$w_s$ ($\mu m$)</th>
<th>$w_v$ ($\mu m$)</th>
<th>$w_h$ ($\mu m$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>48</td>
<td>120</td>
<td>72</td>
</tr>
<tr>
<td>3</td>
<td>46</td>
<td>100</td>
<td>72</td>
</tr>
<tr>
<td>7</td>
<td>48</td>
<td>88</td>
<td>70</td>
</tr>
<tr>
<td>11</td>
<td>50</td>
<td>80</td>
<td>70</td>
</tr>
<tr>
<td>15</td>
<td>62</td>
<td>76</td>
<td>72</td>
</tr>
</tbody>
</table>

From point to point the widths were found to vary in a range of about $6 \, \mu m$ (i.e $\pm 3 \, \mu m$) and the values given in Table 5.1 are the average values. This variation can be due to a non-uniform irradiation and etching of the sample. Within this range $w_s$ increases significantly only below
Figure 5.6: microscopic enlargements of 004 scans after – (a) 3 μm etch, (b) 7 μm etch, (c) 11 μm etch and (d) 15 μm etch.
a depth of $\sim 10 \mu m$. Thus, the distortion interface remains parallel to the irradiation interface (although slightly shifted) almost up to $10 \mu m$ and thereafter shifts away into the irradiated part of the crystal.

All these topographs have been recorded in the configuration $P$ with the diffraction curve of the unirradiated region (outside the irradiated disc) set at the center of the incident beam\textsuperscript{2}. These topographs have also been recorded in the $Q$ and $R$ configurations by shifting the incident beam towards lower and higher angle sides respectively. Topographs recorded after the $15 \mu m$ etch in the configuration $P$ do not have any contrast in the irradiated region (see Fig.5.8 a). Due to this, the width $w_x$ could not be ascertained from this topograph. However, by shifting the beam towards the lower angle side (configuration $Q$) the distorted zones as well as the lines defining the distortion interfaces appear again in dark contrast (see Fig.5.8 c). The values given in Table 5.1 after the $15 \mu m$ etch were actually measured on this topograph.

The distortion interfaces does not have contrast in horizontal stripes, the strain gradient being orthogonal to the incident plane. However, on rotating the crystal through $45^\circ$ about the surface normal, the distortion interface appears in both the stripes as shown in the microscopic enlargement of this topograph (Fig.5.7).

\textsuperscript{2}A discussion on $P$, $Q$ and $R$ configurations can be found in chapter 4, page 77.
5.1.3 Lattice Expansion

An important finding in GaAs is the expansion of the irradiated lattice, not observed in Si. Such an expansion has been observed in the 004 as well as 113 topographs. The results are presented below.

004 Reflections

Microscopic enlargements of the 004 scans of as-irradiated samples, recorded in Q and R configurations are shown in Figs.5.8(a) and (b) respectively. In configuration R, the irradiated zones lose their contrast, indicating expansion of the irradiated lattice. Similar topographs recorded after 15 μm etch are shown in Figs.5.8(c) and (d). Comparing these with Fig.5.6(d), it is seen that the irradiated region has contrast only in the configuration R. This is a direct evidence of lattice expansion in the irradiated region.

113 Reflections

In GaAs, the Bragg angle $\theta_B$ for the 113 reflection is 26.9°, whereas its inclination, $\phi$, with the surface is 25.3°. Hence the incident beam makes a grazing angle of 1.6° with the surface, and its penetration depth is only 1.5 μm. Consequently, the reflection is quite sensitive to surface topology and surface strains.

A stationary topograph of the as-irradiated sample recorded with a wide incident beam is shown in Fig.5.9. It contains two important features – (a) contrast of the stripes and (b) the shift of the diffracted beam from the irradiated disc towards lower angle side.

Stripe-Contrast In this topograph the stripes have black-white contrast. Since it is a stationary topograph, the angle of incidence varies continuously on the sample surface as shown schematically in Fig.5.10. In the direction of the diffraction vector, the stripe-contrast is black-white on the lower angle side of incident beam. In the next stripe it becomes black with thin white lines on both the sides, whereas in the subsequent stripe towards the higher angle side of the incident beam it is white-black. This indicates inward bending in the stripe region. It may be recalled that such a bending was also observed in Si samples and arises due to lateral expansion of the irradiated zones.

Similar topographs recorded after 11 and 15 μm etches are shown respectively in Figs.5.11(a) and (c). Fig.5.11(b) and (d) are 004 stationary topographs which show the position of the distorted sheet after the respective etches. In these topographs, the stripes do not have any

3the topograph shown in Fig.5.11(d) was taken in configuration Q.
Figure 5.8: Microscopic enlargements of 004 scans in the configurations (a) Q and (b) R of the as-irradiated samples, and (c) Q and (d) R after 15 μm etch.
Figure 5.9: Stationary topograph (Cu Kα radiation) of the as-irradiated sample.

Figure 5.10: A schematic diagram showing the variation of the angle of incidence in stationary topographs. Inward bending of planes in the stripes produces black-white contrast on lower angle side. Contrast reverses on higher angle side due to the same bending.
contrast indicating relaxation of lateral stress from the irradiated region.

**Shift in the Diffracted Beam** In all the 113 topographs, the beam diffracted from the irradiated region is shifted towards the lower angle side of the incident beam. Such a shift implies an expansion of the irradiated lattice. In the topograph of the as-irradiated sample the shift is small and increases as the implanted sheet comes closer to the surface after etching. These shifts, expressed in terms of angle $\delta \theta$, as a function of etch are shown in Table 5.2. The corresponding change in the lattice parameter is also given.

<table>
<thead>
<tr>
<th>Etch (µm)</th>
<th>$\delta \theta$</th>
<th>$\delta a/a$</th>
</tr>
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<tbody>
<tr>
<td>0</td>
<td>95&quot;</td>
<td>0.9 x 10^{-3}</td>
</tr>
<tr>
<td>11</td>
<td>460&quot;</td>
<td>4.4 x 10^{-3}</td>
</tr>
<tr>
<td>15</td>
<td>690&quot;</td>
<td>6.6 x 10^{-3}</td>
</tr>
</tbody>
</table>

### 5.2 Stylus Measurements

In these samples (irradiated with a fluence of $5 \times 10^{12}$ ions/cm$^2$), although the X-ray topographs indicated expansion of the irradiated lattice, it could not be observed in the form...
of surface steps either optically or on the stylus$^4$. However, in samples irradiated with $10^{13}$ ions/cm$^2$, such steps could be seen with a CCD camera connected to a computer screen. A plot of surface heights measured on the stylus is shown in Fig.5.12. It can be seen that the irradiated zones are $\sim 200$ Å higher than the unirradiated stripes.

5.3 Principle Observations

- GaAs crystals are sensitive to the electronic energy loss above a threshold of 12 MeV/μm.

- The distortion interface bends more and more into the irradiated part of crystal (away from the irradiation interface) as one moves towards the implanted sheet.

- Damage in the implanted sheet is quite large. As the sheet approaches the surface after successive etching, the damage is detectable in the form of an out-of-plane expansion of the lattice.

$^4$Stylus is a surface profiler used to measure the height of surface steps. In it, a spring loaded tip scans the surface and drives a piezoelectric transducer as a step is encountered. In the present case its resolution has been 10 Å.
5.4 A Comparative Analysis of Lattice Damage in Si and GaAs

The qualitative nature of strain-fields in 200 MeV Ag$^{14+}$ irradiated Si and GaAs samples is broadly the same. However, in certain aspects the two differ significantly. We consider their similarities and dissimilarities and discuss them in the light of TRIM calculations of the lattice damage and energy loss distributions.

Similarities

Lattice Expansion In both the systems the irradiated region has a tendency of lattice expansion which is related to the lattice damage. Maximum damage occurs in the implanted sheet due to elastic collisions and resulting cascades. Electronic energy loss dominated near surface region also experiences lattice modification. Strain in this region is mainly in-plane which is detected as a strain gradient at the interface. In Si, no out-of-plane strain is observed in this region. From the studies of lattice disorder following low energy implants it is known that the strain in an implanted surface is in-plane at low damage levels and out-of-plane expansion occurs only at high damage levels [7, 51]. This can also be understood from energy considerations. The in-plane strain effectively bends the entire crystal for which the required energy is very low. On the other hand, in the case of out-of-plane expansion the bonds at the interface are actually broken.

Distortion Interface In both the systems the distortion interface separating the distorted and undistorted lattices is not the same as the irradiation interface. Below the surface the distortion interface shifts into the irradiated part of crystal.

Dissimilarities

Sensitivity to Electronic Energy Loss On irradiation with 200 MeV Ag$^{14+}$ ions, only GaAs shows sensitivity to electronic energy loss, the observed threshold being 12 MeV/μm. Thus, the observed distribution of lattice damage in these crystals (see Fig.5.4) deviates a lot from that obtained from TRIM calculations (see Fig.5.1) where it is assumed that the solid is insensitive to the electronic energy loss. In Si, on the other hand, no evidence such a sensitivity has been found and the depthwise damage profile is similar to that given by TRIM calculations. Sensitivity of GaAs to electronic energy loss can be attributed to the following factors—
Figure 5.13: TRIM profiles of electronic energy loss of 200 MeV Ag$^{14+}$ ions in GaAs and Si. At the surface the electronic energy loss in GaAs is $1.5$ times more than that in Si.

**Higher Energy Loss** TRIM profiles of ionization following 200 MeV Ag$^{14+}$ irradiation are shown in Fig.5.13 for the cases of Si and GaAs. At the surface, the electronic energy loss in GaAs is $\sim 1.5$ times larger than that in Si. Damage of lattice has been observed in many systems above a certain threshold of the deposited energy density [19].

**Physical properties** The sensitivity of materials to electronic energy loss depends on properties like the e-p coupling strength, the heat of melting and the thermal conductivity. The energy of electronic excitations is finally transferred to the lattice through e-p coupling and a cylindrical column around the ion trajectory gets heated up. The material becomes sensitive to the electronic excitations if the deposited energy density exceeds its heat of melting. Melting points of GaAs and Si are $1513^\circ$ and $1687^\circ$K respectively, while the specific heat of GaAs is $\sim 3$ times smaller than Si at all temperatures [70, 71]. Thus, the threshold is expected to be low in the case of GaAs.

**Damage in the Implanted Sheet** Upon irradiation with ions of same energy, the total lattice damage in the implanted sheet caused by the elastic collisions is much larger in GaAs than in Si. In GaAs samples irradiated with a fluence of $10^{13}$ ions, the damage is so much
that the entire irradiated region rises \( \sim 200 \, \text{Å} \) above the surface. In Si samples, on the other hand, no such expansion has been observed either topographically or by any other technique employed in the present investigations. The larger damage in GaAs can be attributed to higher elastic energy loss in these crystals.