Chapter 2

Crystal Surfaces, An Introduction

Surfaces can have a major, and often detrimental influence on device performance. Their electronic properties can be easily influenced by external parameters, which need to be carefully controlled to achieve device stability and desired device efficiency.

Surface properties depend to a large degree on the crystallographic orientation of the surface, its morphology, the specific defect structure, and its coverage with layers from the ambient. We will first discuss the ideal surface, which can be obtained either by epitaxial deposition, layer for layer, or by the cleaving of an existing crystal in ultrahigh vacuo and consequent passivation.

This chapter is meant to introduce the reader to the general terminology and give a first overview to the surface structural elements. From here, and with the help of experimental evidence described in Chapter 3 we can then proceed to more detailed descriptions of the surface and the related effects.

2.1 The Ideal Crystal Surface

The ideal surface is defined by a clean termination of the lattice at a plane of chosen orientation, and a removal of all atoms at the other side of this plane while leaving the atoms at the lattice side in their original, unchanged position.

Because of the missing attractive forces from the removed atoms, however, there will be some shifting of atoms at and near the surface due to the relaxation of their atomic positions.

In addition, the strong covalent forces in semiconductors will tend to restore some of the broken bonds (i.e., dangling bonds) by reordering of the surface atoms and their bonding configuration in order to minimize the surface energy, and, for covalent crystals, the density of dangling bonds. The process is similar to the reconstruction of
dislocations discussed in *Volume 1*; the *reordering* of surfaces when resulting in a different surface geometry is called surface *reconstruction*. For example, in (111) surfaces of Si crystals, the reconstruction leads to a two-dimensional superstructure, the specific symmetry of which depends on the annealing condition (Schlier and Farnsworth, 1959—see below and Chapter 4).

The ideal surface is unstable. Even the relaxed, but unreconstructed state can only be obtained when stabilizing means are applied. In the above mentioned example of an Si(111) surface which can be obtained by cleavage, reconstruction immediately takes place, even when cleaving in $10^{-10}$ torr vacuum and at 4.2 K (Northrup and Cohen, 1982). Stabilization of an unreconstructed surface can be done, e.g., by saturation of the surface dangling bonds with hydrogen (e.g., using an HF-etch as indicated in Section 2.4.2—Higashi et al., 1990).

### 2.1.1 Crystallographic Aspects, Surface Structures

An ideal crystal surface is described by its Miller indices (as discussed in *Volume 1*). Most surfaces of technical interest are low-index surfaces.

One way of producing such surfaces is by cleaving. *Cleavage planes*, i.e., planes which appear when the crystal is exposed to strong pressure from a knife's edge, are low-index surfaces. These planes have a high packing density within the plane, and show a larger distance to the adjacent plane. They are best defined by internal cohesive forces within each plane, and split more easily from an adjacent plane.

Each semiconductor has its own preferred cleavage plane, such as the (100), (110) or (111) plane. An example of such a surface is the Si(111) surface shown at the top of Fig. 2.1. In GaAs it is the (110) plane which is discussed later.

In order to identify the surface as an unreconstructed one and having the same periodicity of its lattice as the bulk within this surface plane, we add the periodicity identifier $1 \times 1$ behind the denotation of the surface, e.g., here, Si(111)$1 \times 1$ (for more on surface denotation, see Section 2.2.1A).

#### 2.1.1A Surface Relaxation

A cut as shown in Fig. 2.1 leaves the top three rows of atoms without attracting forces from the now missing adjacent atoms. As mentioned before, their relative configuration can be stabilized by saturating their dangling bonds with hydrogen