

PRIORITY COMMUNICATION

A “ROUGH HEART” MODEL FOR “EDGE” DISLOCATIONS WHICH ACT AS PERSISTENT GROWTH SOURCES

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The reason why “edge” dislocations can act as persistent growth sources on Si and GaAs surfaces is thought to be due to the absence of surface reconstruction at a dislocation outcrop. This locally creates a rough surface area where the nucleation rate and growth rate are much higher than on the surrounding surface. In this way a growth hill will develop. When the hill is large enough and stretches beyond the influence sphere of the stress field of the dislocation, its rim will be subject again to reconstruction generating in this way new steps. This mechanism will be especially operative on {001} surfaces of Si and GaAs, although a similar mechanism might also be present on the {111} and {110} faces of these and other crystals belonging to the zincblende structure.

So far in crystal growth theories the only possibility for a persistent step source was the screw dislocation which emerges at a crystal surface emitting growth spirals. Recently Bauser and Strunk [1] have presented convincing experimental evidence that also the outcrop of an “edge” dislocation, that is a dislocation with its Burgers vector parallel to the surface, can act as a point of repeated nucleation. In this way growth hillocks with concentric steps are formed on the {001} surfaces of GaAs.

That such “edge” dislocations are able to function as persistent step sources has also been observed on NaCl and KCl by Keller [2]. This phenomenon is important for all crystal growers, because it gives a fundamental extension to the possibilities for crystal growth.

The question is how to understand its mechanism. Bauser and Strunk give an explanation in which the “edge” dislocation splits into two partial dislocations, generating in this way a stacking fault with compensating components of the Burgers vector normal to the surface. This certainly is a possibility and careful examination of the dislocation and the surrounding step pattern might give more evidence for this mechanism. However, it is not clear why the dislocations should split up and

whether this is a main phenomenon for “edge” type dislocations. In our opinion this explanation is worthwhile to consider but deserves further experimental attention.

Frank, as the father of the growth spiral, has put forward the idea [3] that nucleation is facilitated on one of both stressed sides of the “edge” dislocation, viz. on that side (compressive or repulsive) where the lattice spacing of the nucleus fits best with the local surface spacing. The disadvantage of this possibility is that effectively the action of such a source can only be discerned in a very narrow supersaturation region. The preferential nucleation can only be observed between the $\Delta\mu$ value for the local optimal condition of nucleation and the critical $\Delta\mu_{\text{normal}}$ value for the normal two-dimensional nucleation on the common surface around the dislocations. For, when $\Delta\mu \geq \Delta\mu_{\text{normal}}$ the majority of the growth nuclei will be due to two-dimensional nucleation and these will largely outnumber the nuclei formed on “edge” dislocations. As the reported “edge” sources seem to be quite common and not critical to supersaturation, Frank’s suggestion seems to be questionable.

Fruitful discussions on this subject during the 1983 School on Crystal Growth (ISSCG-5) in

Davos stimulated the idea that a logical explanation of this problem could be given if surface reconstruction is taken into account. For surface scientists who are familiar with surface reconstruction and crystal growth theory the explanation is straightforward and even quite simple.

Surfaces in general constitute a special phase of the solid and from surface detection techniques it is known that the atomic arrangement in the surface top layer can deviate rather drastically from the bulk positions. A special reconstruction exists for the $\{001\}$ surface of Si, Ge, diamond and most of the III-V's including GaAs, which all crystallize in the zincblende or diamond structure.

If such a crystal is cleaved along a $\{001\}$ face and one does not allow (hypothetically) for an atomic readjustment in the top layer, the surface will look like the one pictured in fig. 1. Every atom on the surface has two dangling bonds and such a surface is in essence a rough surface [4]. Each position offers a kink place and every growth unit (e.g. a Si atom) that arrives from the gas phase immediately finds a half crystal place (or a kink position) on the surface and is incorporated in the solid without the necessity to diffuse over the surface to a step or to a kink position in a step. In other words, on such a surface full of kinks a normal growth mechanism is active.

In reality, relaxation of the surface will occur as is always observed for Si, GaAs and related compounds during growth by molecular beam epitaxy (MBE) [5]. The reconstruction on the $\{001\}$ surface is characterized by the dimer formation between

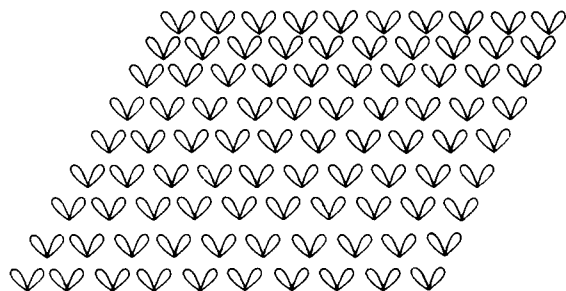


Fig. 1. Unreconstructed $\{100\}$ surface of zincblende type crystals. Each surface site has two dangling bonds. In terms of crystal growth theories such a surface is rough, with a corresponding high growth rate.

adjacent side lobes. This is called a (2×1) reconstruction as the unit surface cell now consists of 2 atoms (fig. 2). This bond formation is rather stable and is observed both for silicon and gallium arsenide up to the growth temperatures (1160 and 620°C, respectively) [5,6]. For GaAs the dimers are formed by the dangling bonds of the As atoms. Therefore, the presence of the reconstruction also depends on the partial pressure of mono-atomic arsenic; higher pressures stabilize the 2×1 dimer formation to higher temperatures. An important point is that the reconstructions are only detectable so far by vacuum techniques (electron microscopy, RHEED, LEED, etc.). Adsorption processes, which can destroy the dimerization, play a minor role in such a high vacuum because of the low concentration of background impurities. Under normal crystal growth conditions adsorption processes can be more severe, because of the high partial vapour pressures. However, it appears that at the growth temperature the adsorption, even at 1 bar, is strongly reduced due to the $T\Delta S$ term in the Gibbs free energy associated with adsorption [7]. Indeed there are positive reasons to believe that also under normal growth conditions of silicon and GaAs by CVD and MOCVD and of GaAs by LPE, adsorption is so small that the (2×1) reconstruction is present at the surface.

The main argument to support this idea is the experimentally observed F-character of the $\{001\}$ face, i.e. the $\{001\}$ face is a stable or flat face. On this surface steps can be found by microscopic methods and even square hillocks and etch pits

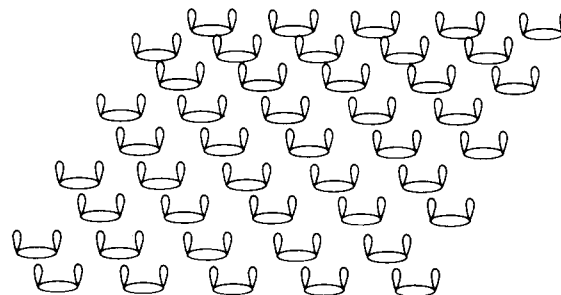


Fig. 2. (2×1) reconstructed $\{100\}$ surface of zincblende type crystals. The alternating reconstruction pattern creates an extra periodic bond chain in the surface. In this way the surface is stabilized and growth will occur by a step mechanism.

have been observed. Also in the plot of the growth rate versus the orientation a cusp occurs in the $\{001\}$ direction [8], showing that this direction has a lower growth rate than adjacent orientations. This is in contrast with what one would expect for an unreconstructed $\{001\}$ surface. Such a face is not flat at all, it is a rough (stepped/kinked (S/K)) face and no steps should be present at all. Instead of square hillocks and pits only a rough surface should be visible. This is in sharp contrast with all experimental observations and gives a strong indication that the $\{001\}$ surface is stabilized by some mechanism. The (2×1) surface reconstruction offers this possibility because it creates an extra periodic bond chain to the one which already exists. In this way it can change the S/K character of the face into an F-one. This idea, which has been presented at the 1983 International Conference on Crystal Growth (ICCG-7) in Stuttgart will be the subject of two forthcoming papers [9,10].

When one accepts that the $\{001\}$ surface of diamond-like crystals is reconstructed under normal crystal growth conditions, the explanation that "edge" dislocations can act as growth sources for concentric steps is rather simple.

When an "edge" dislocation emerges at a $\{001\}$ surface the stress field around the dislocation will locally destroy the (2×1) reconstruction, probably on the repulsive side. Thus at this side of the dislocation a rough area, "a rough heart", will be created, surrounded by a flat stabilized area (fig. 3). Such a local rough area has a higher growth rate than the flat reconstructed surface around the dislocation, and so it will start to grow out normal to the surface. After a few atomic layers it will also spread laterally because the rim also offers kink sites. The centre of the nucleus will remain rough under the stress field of the dislocation, but as soon as the lateral spreading is far enough away from the centre, reconstruction of the atoms of the newly formed $\{001\}$ layers will set in again and steps will be formed.

This mechanism will be operative already at low $\Delta\mu$ because the critical nucleus size is one atom on such a rough surface. The essential difference with Frank's model is that now nucleation is not a rate determining step.

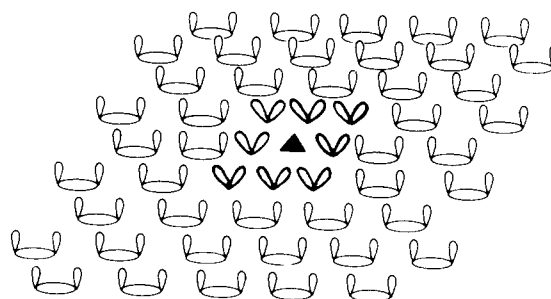


Fig. 3. Schematic idea of the "rough heart" model. Around the dislocation outcrop (▲) the dimer formation is broken, creating a local rough spot on an otherwise flat, reconstructed surface. Locally the growth rate will be higher which gives rise to a persistent step source.

Proof of the reconstruction mechanism should be obtained by looking more closely at the exact centre of the growth hillocks where no steps should be present. From the photographs as published by Bauser and Strunk [1] an indication in this direction can be obtained because in the centre of the growth hill no steps can be discerned. However, the decoration technique could fail to reveal steps there because of the smaller step distance. So a direct proof is still missing, but this must not be too difficult to obtain.

The above mentioned mechanism is not restricted to the $\{001\}$ surface, in fact all surfaces which reconstruct ((2×1) - $\{111\}$, (7×7) - $\{111\}$, etc.) will provide local spots where the reconstruction is destroyed resulting in a higher growth rate. Because of the lack of knowledge about the precise atomic structure of these reconstructions, it is not clear up to now whether here also rough areas will be formed where a critical nucleus of one atom exists. If not, then we end up with the same situation as sketched in the stress model of Frank, viz. that only in a very narrow $\Delta\mu$ range the effect will be observable.

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