Room temperature STM measurements of $\alpha - Ga$ (010)

The STM measurements of $\alpha - Ga$ (010) in the room temperature phase were performed with the room temperature scanning tunneling microscope described in detail in Chapter 2. Due to its low melting point a constant cooling of the $\alpha - Ga$ sample is needed to prevent its accidental melting and subsequent contamination of the UHV system. For this purpose a vibrationless Peltier element was used. The design of a four stage Peltier element is shown in *Fig.39*. Peltier elements are available in the single-stage, double-stage, or multi-stage (3 or 4 stages) design.

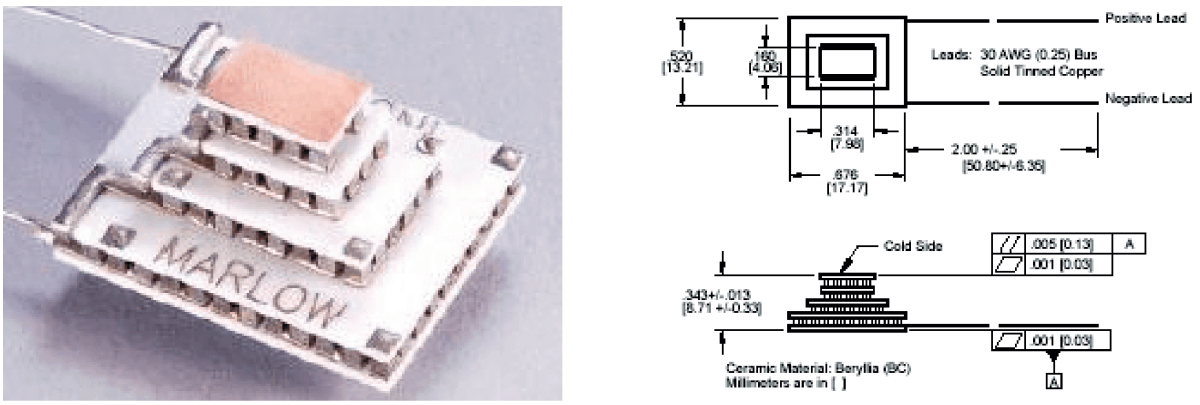

Fig.39
Photography and mechanical characteristics of the Peltier element.

The Peltier element itself can be described as an active heat pump which can be used for heating as well as for the cooling purposes. The working principle of the Peltier element consists in the heat absorption and emission at the contact area of the two conductors of different materials if a current flows through this connection. The quantity of heat absorbed or produced is proportional to the current flowing through the contact. The Peltier effect is especially effective if the contact area is formed by semiconductors of different conductivity. For this alloys of Bismuth and Tellurium doped with Selenium are used. After a complex cleaning and subsequent treatment, one finally receives a polycrystalline material with anisotropic thermoelectric characteristics.

It is of an advantage that such cooling elements have relatively small size and weight, high reliability, a good temperature control and most important for STM measurements that they are vibrationless since there are no moving parts. The data sheet of the used Peltier element

states a maximum temperature difference between hot and cold side of 120°C. The final temperature depends upon the heatload which is here the complete scanner together with the sample. The Peltier element has an efficiency of about 20%, the produced heat flows out of the chamber through a copper rod (20 mm diameter) which is cooled by air. The scanner temperature was typically kept between –10° C and +10° C, well below the melting temperature of $\alpha - Ga$.

Preparation of $\alpha - Ga$ (010) for the room temperature measurements

In this section a number of preparations of the $\alpha - Ga$ (010) surface in the room temperature phase are shown, a more extensive discussion of the sample preparation can be found in the preceding section. *Fig.40 (left and middle images)* shows the $\alpha - Ga$ (010) surface two days after a preparation, while the sample was kept at +10°C. Surprisingly one can still observe big flat terraces and steps which show only small amounts of adsorbates showing that the surface is rather inert. The right image was taken *(Fig.40)* after a preparation with 30 min sputtering (2 keV, Ne gas, $5x10^{-6}$ mbar). Sputtering started at room temperature, then the sample was cooled to 0° C, and finally it was cooled to liquid nitrogen temperature. As a result of such a preparation one can observe narrow terraces and steps pinned at defects. This preparation indicates that the cooling and subsequent warming up for the measurement can result in a roughening of the surface, possibly depending also on the speed of the temperature change.

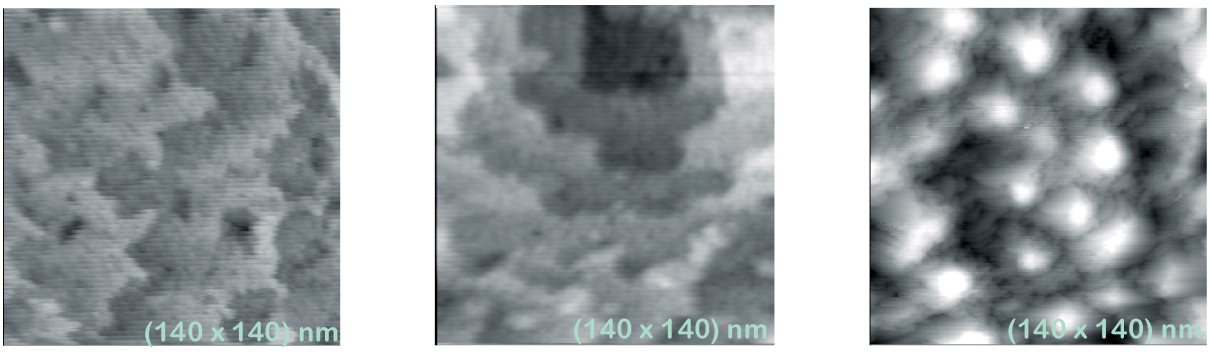

Fig.40

Left and middle images: $\alpha - Ga$ (010) surface after two days without sputtering

Right image: The result of 30 min sputtering (2 keV, Ne gas, $5x10^{-6}$ mbar). Sputtering started at room temperature, then the sample was cooled to 0° C, and finally it was cooled to liquid nitrogen temperature.

In *Fig.41* one can see the result of another preparation (30 min sputtering with Ne gas at 1 keV, and $5x10^{-6}$ mbar). Big flat terraces and steps prolongate essentially in one preferable direction. Areas with straight steps are also observed, proving that the surface of $\alpha - Ga$ is ordered to a high degree. The terraces are not completely smooth, but show some randomly distributed holes and small clusters. By taking images in the same area for a long time, one can see that the surface is not changing. This means that there is no diffusion on the surface once the Ga atoms found their place. This extraordinary thermal stability close to the melting point was found first by [14].

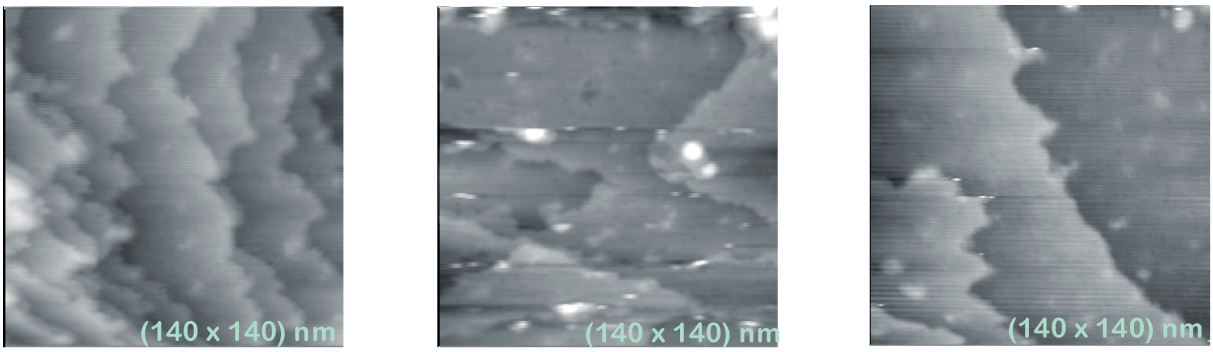

Fig.41
The result of a preparation with 30 min sputtering with Ne gas at 1 keV and $5x10^{-6}$ mbar. One observes big flat terraces and steps prolongating essentially in one preferable direction.

In *Fig.42* one can see the result of a sample preparation identical to the preparation described above (30 min of sputtering with Ne gas at 1 keV, and $5x10^{-6}$ mbar). One still observes big flat terraces and steps prolongating in the preferable direction and also perpendicular to it. The fact that one can observe straight steps and also the 90° angles proves the good state of the surface. Again holes and clusters are present on the terraces. Other preparations showed more disorder and resembled the surface achieved for the low temprature measurements (*Fig.47*).

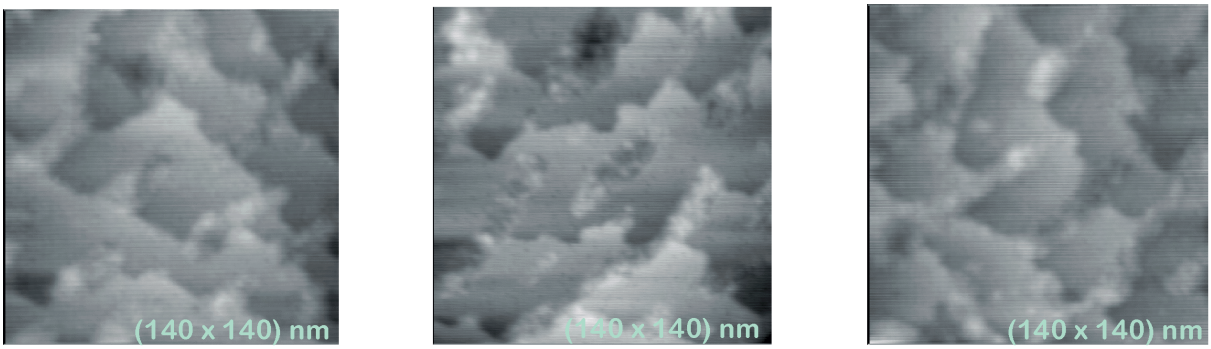

Fig.42

The result of the sample preparation identical to the preparation as in Fig.41 (30 min of sputtering with Ne gas at 1 keV, and $5x10^{-6}$ *mbar). One still observes big flat terraces and steps prolongating in the preferable direction and perpendicular to it.*

Common in all these preparations is that they show steps of equal height. The measured height of the step is always $3.8\,\mathring{A}$ corresponding to the interdimer distance in the bulk. The linescans showing the step height are shown in *Fig.43*.

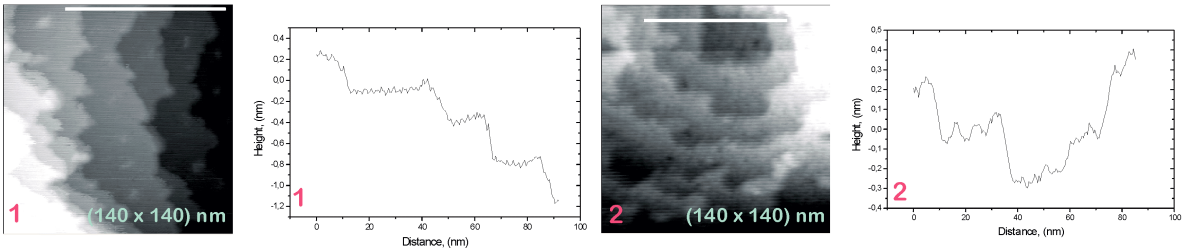

Fig.43

Two topography images with the corresponding linescans. The lines of the 1-d-scans are marked with a white line.

Steps with a height of $1.9\,\mathring{A}$ were never found, which is the same result as in the low temperature phase. The single step heigth means that there is only one termination possible on the surface: A, B, or C termination. This result is in accordance with [14] shown in *Fig.43*. A step heigth of $1.9\,\mathring{A}$ would result from single atom layers, so Ga_2 dimers can be considered as the building blocks of the crystal.

At this point room temperature STM results for the $\alpha - Ga\,(010)$ surface from Züger and Dürig (ZD) [14] will be compared with the results obtained in this work. ZD obtained their

STM images of the sputter cleaned surface by a lock-in method due to difficulties in the normal image mode. The gradient image $\partial z / \partial x$ calculated from individual line scans is displayed to enhance the visibility of the steps (*Fig.44, left image*). The surface consists of remarkably large terraces $\left(1000\,\mathring{\mathrm{A}}\right)$ separated by irregulary oriented step lines. The presence of such large, atomically flat terraces is surprising, because the surface was sputtered with 2 keV Ne^{+} ions. Surface defects (holes, vacancies, adatom clusters) induced by the sputter-cleaning process are completely absent. Post-sputtering annealing of the defects by surface diffusion would be one explanation of their absence. However, surface diffusion was never observed in STM images, measured up to the onset of the bulk melting.

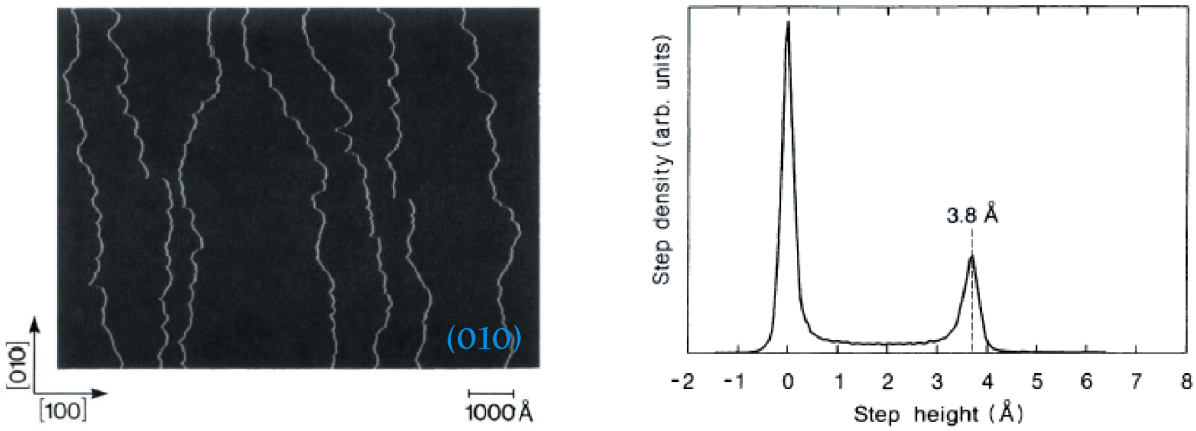

Fig.44

STM images obtained by Züger and Dürig [14] with a lock-in method and a histogram of step-height distribution from this image.

In contrast, the STM images of this work show terraces containing holes and clusters, but also partly straight steps, while the Züger and Dürig work shows ideal defect-free terraces but irregulary oriented steps. Straigth steps and right angles are formed in case of a clean surface and sufficient mobility. The holes and clusters on the terraces are formed during sputtering, the subsequent resting time allows then an ordering process. Defects were still present upon reduction of sputtering energy and sputtering gas pressure. Therefore the sputter energy cannot explain the difference in surface quality between ZD and the present work.

Atomic resolution

In *Fig.45* one can see the atomically resolved image of the room temperature phase of the $\alpha - Ga$ (010) surface obtained with the lock-in method by Züger and Dürig [14].

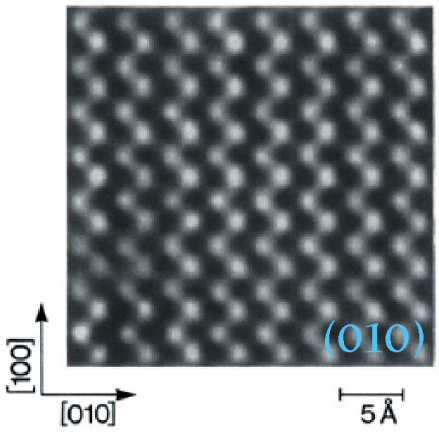

Fig.45

Atomic resolution image of the $\alpha - Ga$ (010) surface obtained by using a lock-in technique. The image shows (1x1) structure [14].

Züger and Dürig did not succeed in achieving atomic resolution in the normal imaging mode. In the present work difficulties with obtaining the atomic resolution images of the room temperature phase of $\alpha - Ga$ were faced, because of a 5 Hz noise from the thermal connection between the Peltier element and the scanner. These circumstances made a number of instrumental changes necessary. First of all, the scanner was attached to the base plate. By doing so the eddy current dampers and springs were not needed any more (*Fig.46, upper images*). The high stability of the scanner allowed to work without a damping of the acoustic noise. The changed setup was checked with a Ag (001) single crystal (*Fig.46, lower images*).

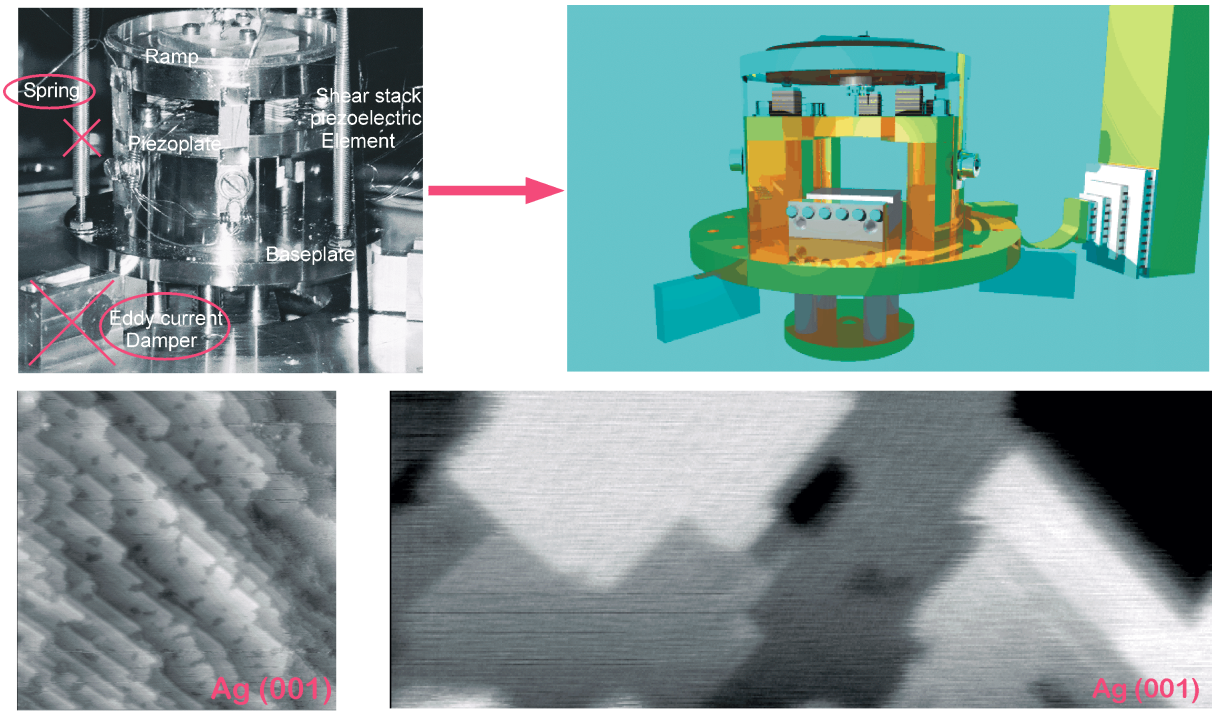

Fig.46

Changed scanner setup and Ag (001) test images.

These images show that the scanner is working well without eddy current dampers and a resolution of less than 0.01 nm was achieved. The scanner was thermally isolated from the base plate by using only stainless steel components with a low thermal conductivity. After the instrumental changes the work with the Ga sample was continued.

The crystal was prepared in a usual manner with Ne gas sputtering at 1 keV for about half of an hour. Care was taken to switch off the ion gauge in the preparation chamber during all the cleaning procedure to prevent heating of the sample. The result of this preparation can be seen in *Fig.47.*

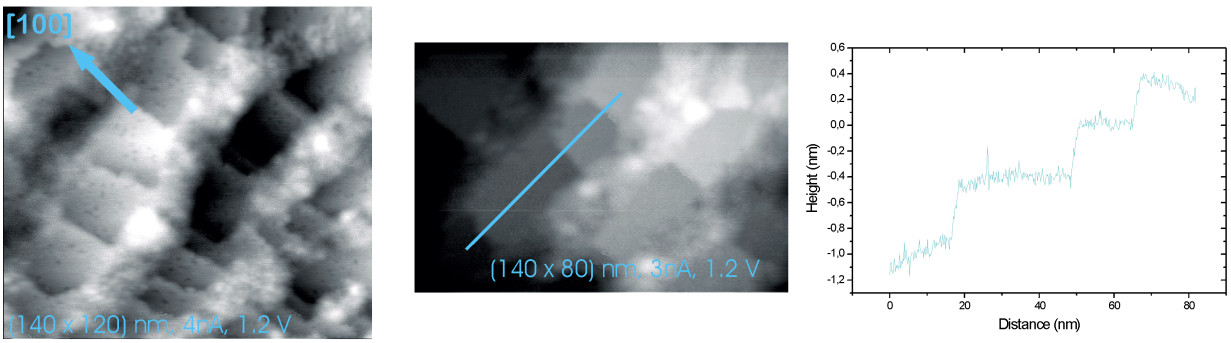

Fig.47

Big scale image of the room temperature phase of the $\alpha - Ga$ (010) surface and a corresponding linescan.

In *Fig.47* one can see big flat terraces and steps which run along the [100] glide plane direction. One can also observe 90° angles in these images. This proves that the surface is in a good state. A linescan performed in the middle image of *Fig.47* again shows the standard step height of 0.38 nm. Terraces are flat and exhibit holes which point also into the direction of the glide plane and perpendicular to it (see *Fig.48*, left image).

As a result of this preparation, atomically resolved images were routinely obtained on the clean areas of the terraces. The atomic resolution images show `zigzag` rows which run in the glide plane [100] direction. The atomic resolution was checked by rotating the scan direction, thereby excluding electronic noise as the source of the surface appearance. The corrugation in these images is of the order of 0.01 nm, which is comparable to the estimate from the Züger and Dürig lock-in measurements. The appearance of the atomically resolved surface structure is tip dependent, but also can change across the terrace due to surrounding defects. These images represent the first truly atomically resolved STM images of the Ga surface.

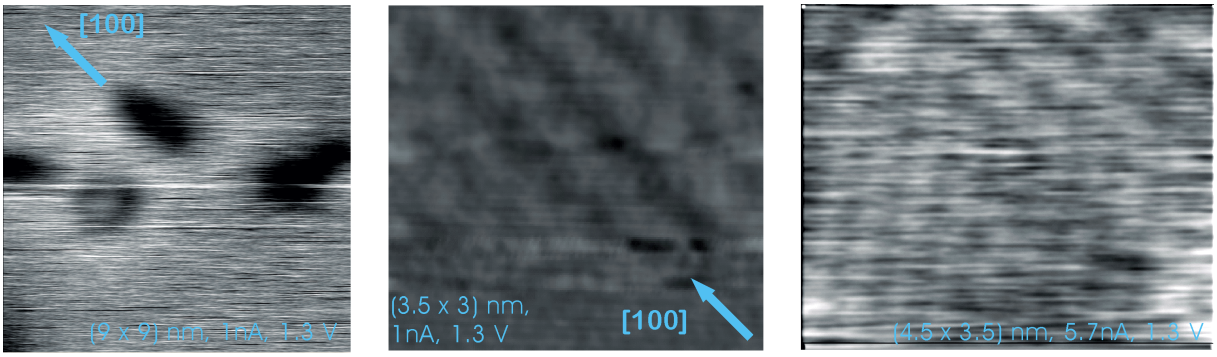

Fig.48

Left: Holes on $\alpha - Ga$ (010) surface are pointing in the direction of the glide plane and perpendicular to it.

Middle and right: Atomically resolved images of the room temperature phase of $\alpha - Ga$ (010) show `zigzag` rows running along the glide plane [100] direction.

Ga facets

Next to the atomically resolved terraces a number of facets were resolved. The images in *Fig.49* and *Fig.50* show the atomically resolved 2D, 3D and high pass filtered images of a pyramid of Ga atoms on the $\alpha - Ga$ (010) surface. Each side of the pyramid exhibits another facet. The height of the pyramid is 3.25 nm which equals to 8 layers of Ga dimers.

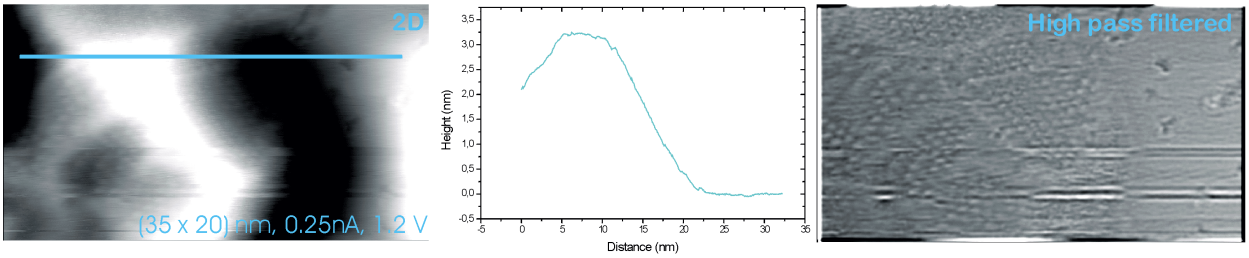

Fig.49

The pyramid of Ga atoms: 2D and high pass filtered images. The corresponding linescan shows that the pyramid height equals to the 8 layers of Ga dimers.

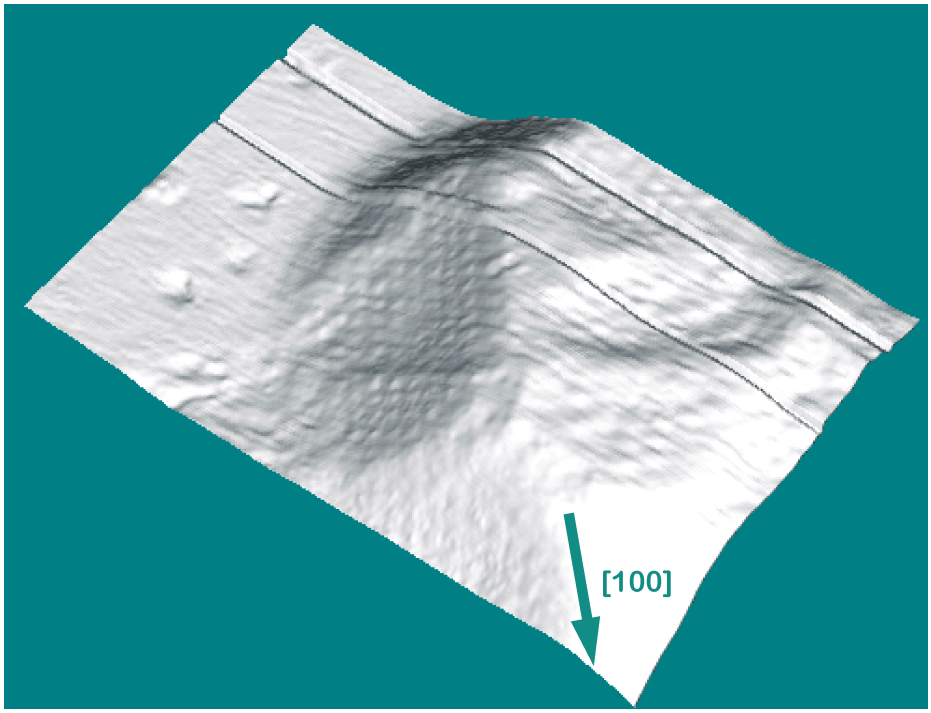

Fig.50

3D image of the atomically resolved pyramid of Ga atoms on $\alpha - Ga$ (010) surface.

A similar structure was obtained during the measurements of the low temperature phase (*Fig.51*). One can clearly see that this one-domain area has nothing in common with the usual two domain stripe-like structure of the low temperature phase of $\alpha - Ga$. This shows that the observed facets do not undergo a phase transition.

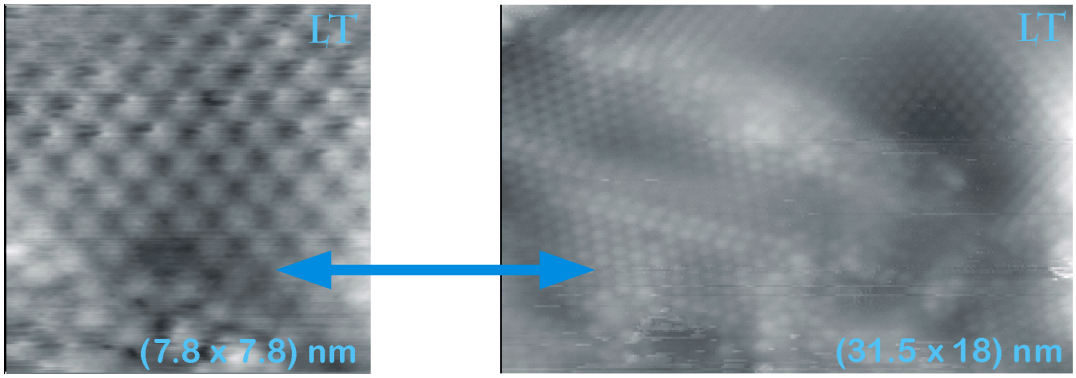

Fig.51

Left: Atomic resolution image of a facet on the $\alpha - Ga$ surface.

Right: Exceptional one-domain area obtained by the low temperature STM measurements.

Calculations

For a further clarification of the low temperature phase, tight binding calculations were performed. For this a tight binding calculation program of J. Cerda [16] was used, allowing band structure calculations for surfaces as well as STM simulations. The surface band structure of termination B obtained with this program (*Fig.52, left image*) is in a good agreement with LDA calculations made by Bernasconi (*Fig.52, right image*) [7].

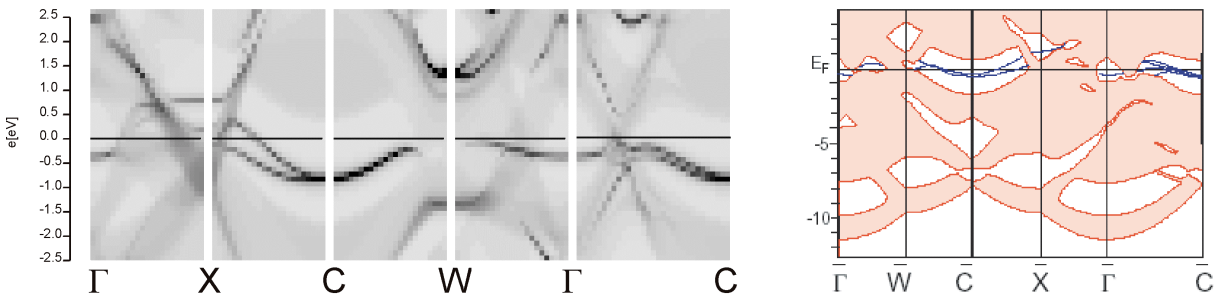

Fig.52

Surface band structure of the Termination B.

The topographic STM images were calculated for the termination B for the low temperature phase (*Fig.53, left image*) and room temperature phase (*Fig.53, right image*) correspondingly. Both of the simulations for the low and room temperature phases were done with a Pt tip with a four atom pyramid at the tip apex. In these calculations the bulk is set to be semi-infinite. So below the topmost surface layer there is a semi-infinite Ga bulk with the well-known bulk structure. For the topography STM calculations a current of 1nA and voltage of 100 mV was used. Depending on the resolution such a simulation takes between 10 and 60 minutes on a regular PC.

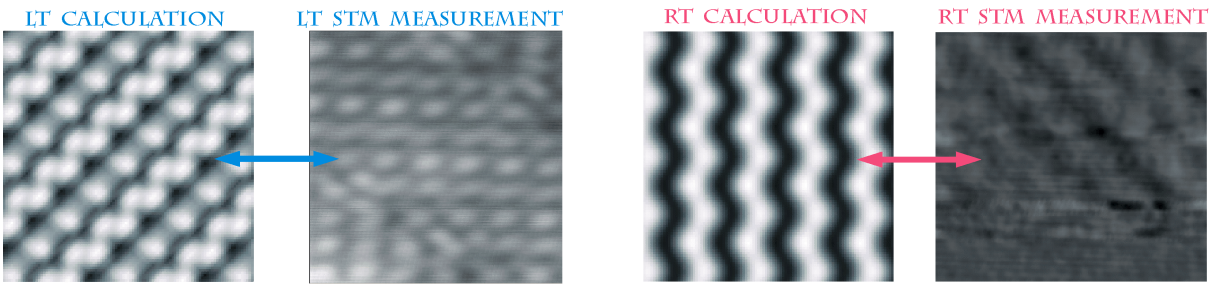

Fig.53
Left: Comparison of the structure calculation for the room temperature phase and LT STM measurements.
Right: Comparison of the structure calculation for the low temperature phase and RT STM measurements.

Comparison of the calculated images with the experimental data shows good agreement both in the low temperature and room temperature phase. All the calculations were done with a model with 8 atoms per unit cell as present in the Termination B.

For the agreement with calculations the intuitive model of the low temperature phase structure (*Fig.54, left image*) needed to be changed. The changes are a rotation of the inner dimer row. So the `bump` row consists of dimers pointing in the same direction but with alternating heights of the dimers (red colour is higher than blue color). The `zigzag` row consists of dimers pointing in the perpendicular directions, but positioned at the same height.

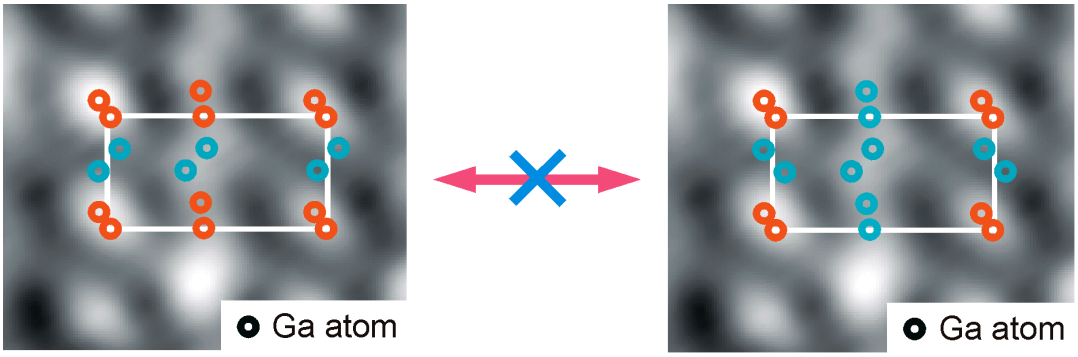

Fig.54

Left: Intuitive structural model on the basis of the STM measurements.

Right: Corrected structural model on the basis of the topography calculations.

One can see the changed structure model in the right image of *Fig.54*. There the first and third rows are the `bump` rows and the second row is a `zigzag` row. For a final structure clarification LDA calculations should be employed.

Conclusion

Low temperature STM and room temperature STM investigations of the Ga(010) surface have been performed within this work. Here the surface has been imaged for the first time in the low temperature phase with scanning tunneling microscopy. The surface shows two domains which form well ordered parallel stripes. The unit cell was investigated in detail and a structural model is proposed. The presence of a charge density wave is not expected apriori on the Ga(010) surface, but was identified unambiguously with tunneling spectroscopy. With the normal imaging mode the atomically resolved structure of the room temperature phase of Ga was imaged for the first time in the present work.

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