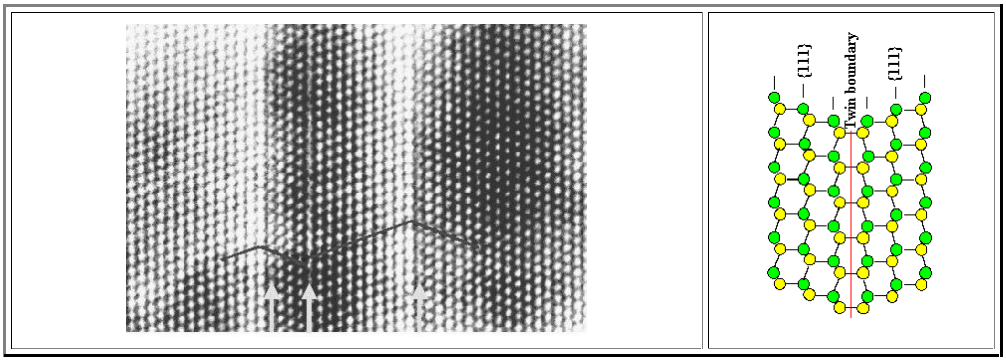
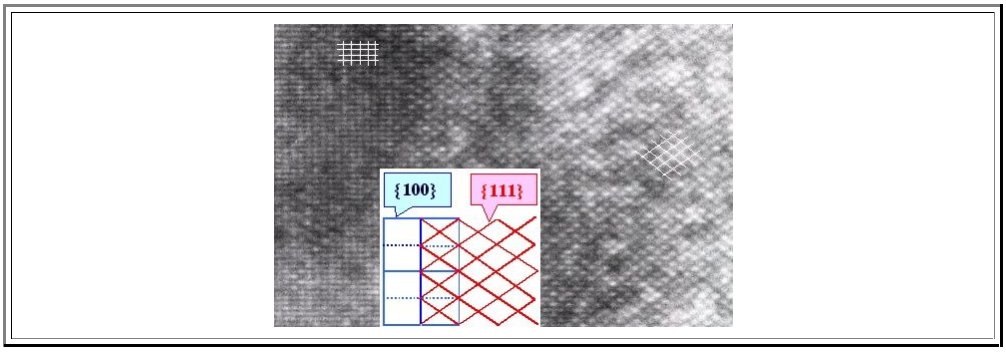
6.3.4 High Resolution TEM

- High-Resolution **TEM** (***HRTEM***) is the ultimate tool in imaging defects. In favorable cases it shows directly a two-dimensional projection of the crystal with defects and all.
  - Of course, this only makes sense if the two-dimensional projection is down some low-index direction, so atoms are exactly on top of each other.
- The basic principle of **HRTEM** is easy to grasp:
  - Consider a very thin slice of crystal that has been tilted so that a low-index direction is exactly perpendicular to the electron beam. All lattice planes about parallel to the electron beam will be close enough to the Bragg position and will diffract the primary beam.
  - The diffraction pattern is the **Fourier transform** of the periodic potential for the electrons in two dimensions. In the objective lens all diffracted beams and the primary beam are brought together again; their interference provides a back-transformation and leads to an enlarged picture of the periodic potential.
  - This picture is magnified by the following electron-optical system and finally seen on the screen at magnifications of typically $\mathbf{10^6}$.
- The practice of **HRTEM**, however, is more difficult them the simple theory. A first illustration serves to make a few points:



  - The image shows one of the first **HRTEM** images taken around **1979**; it is the **<110>** projection of the **Si**-lattice; a schematic drawing is provided for comparison. It also contains a few special grain boundaries, called twin boundaries.
- We notice a few obvious features:
  - Instead of two atoms we only see a dark "blob."
  - Or does the dark blob signal the open channels in the lattice projection? There is actually no way of telling from just one picture.
  - The twin boundaries look fine in comparison to the drawing at a first glance. Looking more closely, one realizes that there are a few unclear points: The yellow arrow points to "fuzzy" lattice planes to the right (or left) of the boundary. Following a fringe across the boundary seems to result in an offset - what does it mean? But what should we expect defects (in this case the twin boundaries) to look like? After all, they destroy the periodicity of the lattice and it is not obvious what Fourier transforms of defects will produce in general cases.
- The last point is easy to solve: Just do a simulation of a defect (i.e. calculate the image for an assumed slice of a crystal with all atoms at the proper positions), but mind the points mentioned below! These are the limitations to **HRTEM** stemming from the non-ideality of the instrument and the specimen:
  - The specimen is not arbitrarily thin! If the thickness is in the order of the extinction length, some reflexes may have very small intensities because they were diffracted back into the primary beam. The objective lens then will not be able to reconstruct the spatial frequencies contained in these reflections; the image looks like a different lattice.
  - This can be nicely seen in a **HRTEM** image of **Si** where the thickness of the sample increases continuously:



- The inset shows the lattice in **<110>** projection; an elementary cell is given by the large rectangles formed by solid blue lines.
- On the right hand side of the picture, all reflections are excited; the very strong **{111}** reflections dominate the image and the **{111}** lattice planes (indicated by white lines) are most prominent. On the left hand side the thickness happens to be in a region where the **{111}** reflections are weak; the **{400}** type reflections dominate (**{100}** etc. are "forbidden" in the diamond lattice). The lattice appears rectangular.

In principle, this can be calculated, too, without much problems. What is much more problematic is the "**contrast transfer function**" of the objective lens.

- If we consider the objective lens to be some kind of amplifier that is supposed to amplifies (spatial) frequencies in the input with constant amplification and without phase distortion, the objective lens is a *very bad* amplifier. It has a frequency response that is highly nonlinear, the amplification drops off sharply for high (spatial) frequencies (meaning short distances). In other word, the resolution is limited (to roughly **0,1 nm** in good **TEMs**); you cannot see smaller details.
- But worse yet, around the resolution limit, the objective lens induces strong phase shifts as a function of several parameters (the most important one being the focus setting); this influences the interference pattern which will define the image.

Both effects together can be expressed numerically in the contrast transfer function of the lens. If you know that function (for every picture you take) you may than calculate what the image would look like for a "perfect" lens with a certain resolution limit; or somewhat easier, you calculate what a crystal with the defects you assume to be present would look like in your particular microscope with the contrast transfer function that it has.

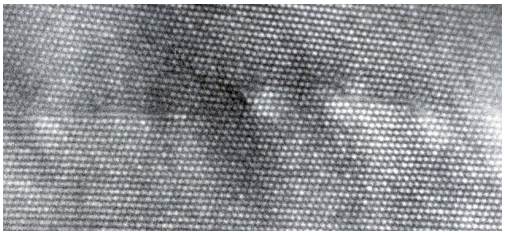
Neither approach is very easy; the amount of computing needed can be rather large. Worse, you must determine parts of the contrast transfer function experimentally; and that involves taking several images at different focus settings. Still, **HRTEM** images provide the ultimate tool for defect studies. They are perfectly safe to use without calculations if you obey two simple rules:

- Only look at pictures where the perfect part of the crystal looks as it should. After all, you usually know what kind of material you are investigating. So if the image of a diamond structure looks like the left part of the illustration above; throw it away (or at least use with care). It it looks like a diamond strucure you can't go totally wrong in interpreting the picture.
- Only draw qualitative conclusions (e.g. there is a dislocation in this **GaAs** specimen!); never draw quantitative conclusion (e.g. it ends at a Ga atom!) without calculating the image.

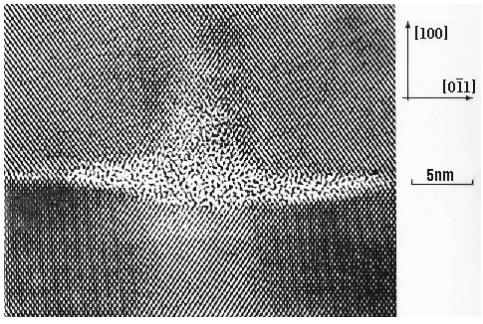
Some more details to **HRTEM** imaging can be found in the (German) article in the link

Three examples may serve to illustrate **HRTEM** here; more will be found in the upcoming chapters.

- The first picture shows a small angle grain boundary in **Si**. This was the first picture of this kind; it only can be interpreted qualitatively; the contrast transfer function was not known. What we see beyond doubt are several lined-up dislocations which constitute a boundary - the top half of the lattice is tilted with respect to the bottom half.

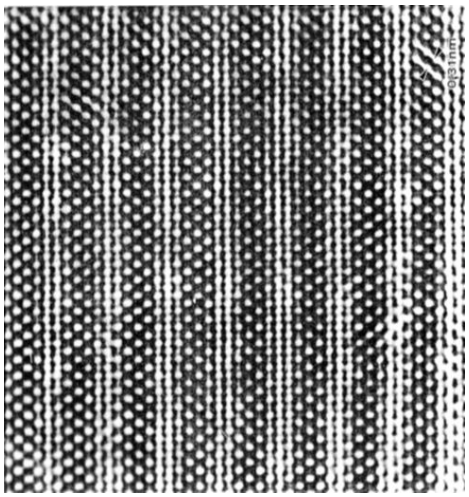


- The next picture (from W. Bergholz) shows an **SiO_2** precipitate in **Si**. Again, a qualitative interpretation is neither possible nor necessary. It is clear that the precipitate, albeit very small, is not spherical



Courtesy of W. Bergholz

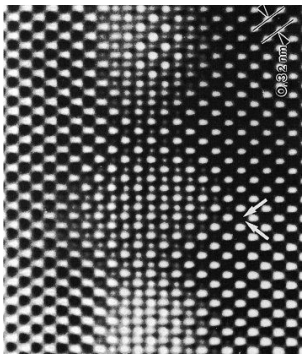
The last example shows quantitative **HRTEM** (from W. **Jäger**) Careful imaging under various conditions, extraction of the contrast transfer function and prodigious computing allowed not only to image a sequence of **Si - Ge** multilayers produced by molecular beam epitaxy (***MBE***), but to identify the positions of the **Si** and **Ge** atoms. The first picture shows an overview. The brighter regions indicate the **Ge** layers, but it is not clear exactly how the lattice changes from **Si** to **Ge**.



Courtesy of W. Jäger

This image also demonstrates the progress made in building electron microscopes. The "old" pictures shown above were taken with a the best general-purpose **TEM** available around **1980** (Siemens Elmiskop **102**). The last pictures were taken with a **TEM** optimized for high resolution around **1995**.

Next a comparison between an enlarged part of the **Ge/Si** stack is shown together with a quantitative evaluation of this and other pictures obtained at different focus settings from W. Jaeger and his group. The color codes defined **Ge** concentrations and a very clear representation of the multilayer sequence is obtained.



Courtesy of W. Jäger