m15.o05

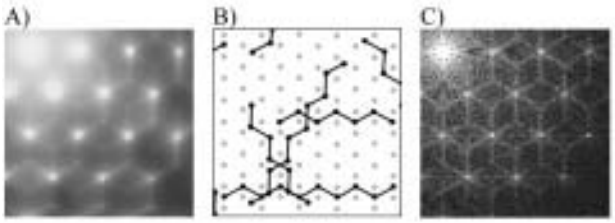
Computer assisted analysis of diffuse electron diffraction of precipitates in GaAs

Holm Kirmse[a], Ines Häusler[a], Irmela Hähnert[a], Wolfgang Neumann[a] and Kurt Scheerschmidt[b]

[a]Humboldt University of Berlin, Institute of Physics, Chair of Crystallography, Newtonstrasse 15, D-12489 Berlin, Germany, and [b]Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle, Germany. E-mail: holm.kirmse@physik.hu-berlin.de

Keywords: diffuse electron diffraction, computer simulation, GaAs

The single crystal growth of GaAs for epitaxial substrates is inseparably correlated with the formation of As precipitates of some nanometers in diameter due to retrograde solubility during cooling of the crystal to room temperature. These precipitates are the origin of diffuse scattering observed as weak lines in transmission electron diffraction (TED) pattern (see Fig. (A)). In order to thoroughly understand the structural characteristics of the precipitates computer simulations of the TED patterns were performed.
Simulations were carried out via two different approaches. In a first simplified assumption 2-dimensional projections of the structure along [111] and [110] were considered. For the evaluation of the agreement between structure model and experimental findings the Fourier transform of the projected positions of the atoms was calculated. The regular positions of the atoms of the sphalerite structure are depicted as grey dots in Fig. (B). The Fourier spectrum clearly exhibits intensity maxima at positions expected for the perfect crystal (see Fig. (C)). In order to generate the diffuse lines in the Fourier spectrum interstitial atoms have to be incorporated. With respect to the ratio of its ionic radii, Ga and As are preferentially incorporated on a 4-fold coordinated site. But, an agreement is found only for the arrangement of interstitials as given in Fig. (B) as black dots. These positions are either the 3-fold or 2-fold coordinated ones which are not distinguishable in this projection. For visualization of the two-dimensional arrangement, the interstitial atoms were connected by lines not contributing to the Fourier spectrum.
In addition to this first approach, simulations of the TED pattern basing on three-dimensional models structurally relaxed by molecular dynamics calculations will be discussed. The findings of the computer simulations will be verified by comparison with results of high-resolution transmission electron microscopy (HRTEM) as well as high-angle annular dark-field scanning TEM (HAADF STEM).



Diffuse electron scattering of precipitates in GaAs: A) part of experimental [111] diffraction pattern, B) [111] projection of atomic positions of sphalerite structure (grey) and additional As atoms (black), C) Fourier spectrum of (B).

m16.o01

Quantitative Characterization of Aperiodic Nanostructures: the Advantage of Using Electrons

Sandra Van Aert

Department of Physics, University of Antwerp, Antwerp, Belgium. E-mail: sandra.vanaert@ua.ac.be

Keywords: electron microscopy, precision, resolution

In science, and in nanoscience in particular, there is an evolution from describing phenomena toward understanding and finally toward predicting. At the same time, there is a steady improvement of quantum mechanical ab-initio methods to compute the physical properties of nanostructures. However, validation and further improvement of these methods are only possible by interaction with experiments. This requires experimental characterization methods yielding local, quantitative structure information with a sufficiently high precision. For this purpose, electrons are most suitable. According to Henderson [1], from all imaging particles, electrons provide the most structure information for a given amount of radiation damage, even several hundred times more information than X-rays. Furthermore, as a result of the strong interaction of electrons with the material under study, it is possible to obtain local structure information, in contrast to, for example, X-rays, which only provide averaged structure information using classical diffraction techniques. For this reason, electron microscopy is expected to provide precise, numerical values of relevant physical structure parameters, such as atom positions, atom types, and locations of spectral peaks. For many materials, their properties change if atoms are moved over a distance of the order of 1 pm or when the bandgap energy changes with 50 meV [2-3]. This means that the precision with which atom positions and locations of spectral peaks have to be measured, should be of the order of 1 pm and 50 meV, respectively. Recent developments in the design of the microscope have improved the spatial and energy resolution to 100 pm and 250 meV, respectively. This allows microscopists to visually distinguish atom columns of solids, projected along a main zone axis, and to visualize the fine structure of electron energy loss spectra. A common misunderstanding is that one is inclined to think that a precision of the order of 1 pm or 50 meV, requires a further improvement of the spatial and energy resolution to 1 pm and 50 meV, respectively, which is far beyond the present possibilities. The reason for this is that structure determination is, up to now, mainly based on visual inspection of the observations. From the point of view of visual inspection, a good resolution is important. Indeed, resolution expresses the possibility to visually distinguish neighboring components in the observations. Precision, on the other hand, is a fundamentally different notion. In order to measure parameters precisely, the availability of a physical model of the observations is needed, which may be adapted to the observations with respect to the unknown parameters. 'Precision' then corresponds to the variance or the standard deviation of the thus obtained measurements of the physical parameters. In fact, an image may no longer be judged by its visual quality, but should be considered as an experimental dataset from which physical parameters have to be measured as precisely as possible. In order to reach this goal, merely visual interpretation of the observations is inadequate. Quantitative, model-based methods are needed.

[1] Henderson R., *Quarterly Reviews of Biophysics*, 1995, 28, 171.
[2] Muller D.A., *Ultramicroscopy,* 1999, 78, 163.
[3] Van Dyck D., *Advances in Imaging and Electron Physics*, 2002,