s10.m32.o2 **Particle Sizing of Tetrahedral and Hemispherical Particles from Small-Angle Scattering Experiments.** Wilfried Gille, *Martin-Luther-University Halle-Wittenberg, Department of Physics, SAS-Laboratory, Hoher Weg 8, D-06120 Halle Germany, E-mail: gille@physik.uni-halle.de*

Keywords: Tetrahedron and Hemisphere; SAS Correlation Function; Ill-Posed Problem

Particle sizing based on measurements of random intercept lengths on a random line through many homogeneous particles embedded in a matrix (isotropic two-phase sample) is a basic stereological problem [1]. Important applications are in materials science and biology beginning at a length scale of several nanometers. The determination of particle size distributions of selected particle shapes from experimental data has already been discussed for a large class of geometric shapes [2,3]. There exist two basic principles of the measurement: On the one hand, particle size distributions of a sequence of well-defined particle shapes can be obtained via pure image analysis [3]. On the other hand, scattering experiments with electromagnetic waves lead to scattering curves, which as well include the information about the particle size [4,5,6].

Basic approaches for a large spectrum of three-dimensional particle shapes (including two-dimensional and one-dimensional limiting cases) are known. Several particle shapes can be handled by use of the so-called Titchmarsh transformation, see [2,6], which allows to determine the size distribution density of a characteristic diameter of the particle analytically, in case that the small-angle scattering (SAS) intensity of a single prototype of particle is proportional to the square of the Bessel function of the first kind of index ν. Unfortunately, analytic solutions based on such special integral transformations are rare exceptional cases. The particle shapes considered here are very special ones and therefore do not seem to have been considered yet in greater detail. The investigations consider so-called *quasi-diluted arrangements* of microparticles. Here, the greatest particle diameter is smaller than the smallest distance between any two particles. The assumptions given are: Analysis of isotropic quasi-diluted polydisperse arrangements of homogeneous tetrahedral or hemispherical particles (two independent and separate cases), independently arranged in space. The tetrahedrons possess a random edge length a and the hemispheres possess a random diameter d.

Approaches for the determination of the size distribution densities $f(a)$ and $f(d)$ via the first principles of random intersections of the microparticles based on the *single particle set covariance* have been explained. Hereby, no assumptions about a special type of the unknown function f (like log-normal-distribution, Rayleigh-distribution) are made. In the first case, the starting point is the application of the averaged isotropized set covariance of a single tetrahedron $C(r)$. Robust and reliable procedures for handling the resulting equations numerically are presented. As $C(r)$ is closely connected with the small-angle scattering correlation function $\gamma(r)$, which in its turn is connected with the SAS intensity, particle sizing via scattering methods of tetrahedral or hemispherical micro objects in materials science and biology can be realized. In fact, the application of scattering methods does not require image material. However, the particle shape must be known *a priori* [7]. This assumption of a quasi-diluted particle arrangement is indispensable for interpreting the SAS experiments. The whole scattering intensity is simply the sum of the scattering intensities of all particles. Describing this averaging step theoretically, the SAS structure functions of the single tetrahedron, see [8,9], and of the single hemisphere (for constant particle size) are the starting point. After performing the averaging procedure with respect to number or size, the theoretical scattering curves of

s10.m32.o3 **Analysis of strain state of semiconductor structures by large-angle convergent electron beam diffraction.** H. Kirmse, I. Hähnert, W. Neumann, *Humboldt University of Berlin, Institute of Physics, Chair of Crystallography, Newtonstrasse 15, D-12489 Berlin, Germany. E-mail: holm.kirmse@physik.hu-berlin.de*

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Convergent beam electron diffraction (CBED) of a sample in off-eucentric height provides information about both the lattice geometry as well as the structural peculiarities of the sample in one and the same experiment (Ronchigrams). Inside the central disc of the zero-order Laue zone the dark deficiency lines are visible corresponding to excess lines in higher order Laue zones (HOLZ). A shift of the position of HOLZ lines while crossing an interface indicates a variation of the local lattice parameters.

This method was applied to two different elastically strained layer systems.

First a 30 nm thick (Zn,Cd)Se layer embedded in ZnSe was investigated with respect to its strain state. The sample was grown by molecular beam epitaxy (MBE) at a temperature of 320 °C. The nominal Cd content was 20 %. Here, the lattice mismatch of about 1.4 % affects an elastic deformation of the ternary layer without formation of defects. Hence, the composition is directly correlated with the lattice constants. Owing to the different lattice parameters of ZnSe compared to (Zn,Cd)Se the HOLZ lines are curved when approaching the

interfaces (see Fig. 1.) The dimension of the region where the HOLZ lines are curved clearly depends on the Cd diffusion length. The positions of the HOLZ lines with respect to composition and lattice parameters were simulated using the Electron Microscopy Image Simulation (EMS) software package. The results are in agreement with findings of TEM diffraction-contrast imaging and energy-dispersive X-ray spectroscopy.
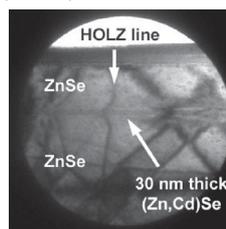
Fig. 1: LACBED pattern of a (Zn,Cd)Se layer embedded in ZnSe.

A second sample was produced by combined use of metal organic vapour phase epitaxy and lithographic structuring of V-grooves. Multiple transitions of strain state from compressive to tensile an vice versa is introduced by materials of different

lattice parameters. The aim of the growth experiments was to neutralize the total strain by capping the tensily strained V-grooved (In,Ga)P with compressively strained GaAs or (In,Ga)P. In Fig. 2 HOLZ lines crossing the different interfaces show an inversion of bending indicating a reversal from compressive to tensile and to compressive again.
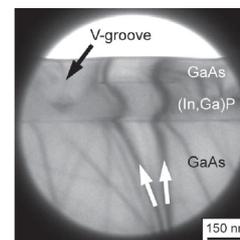

Fig. 2: Bent HOLZ lines in a V-grooved structure.