s8.m27.o5 **An Analytical Approach to the Indexing of Multiphase Powders.** Zlokazov V.B., *141980 FLNF JINR Dubna, Russia, E-mail: zlokazov@nf.jinr.ru*

**Keywords: Powder Indexing; Multiphase Powders; Fitting**

A very important particular case of indexing the multiphase powders is detection of impurities and their inhibiting from an influence on the indexing of the master crystal. To a certain extent the situation is similar to the background suppression in the procedures of line spectrum analysis. Here the impurities play also the role of the background. An analytical approach to the solving of this problems consists in the following.

A diffracted reflection of d-spacing d_exp belonging to the ith phase can be formally described by the function d(P_i,H_i), where P_i is the unit cell parameter vector, and the vector H_i is a triple of Miller indices. So given a set S = (d_k), k=1,2,..,m, their errors (err_k), and the symmetries of the phases we can formulate the main problems of the indexing: fit the data (d_k) by the functions d(P_i,H_i), considering the quantities P_i and H_i as parameters.

The problem of such fitting is strongly non-linear, and has no analytical solution, but in particular cases it can be solved, using an approximate algorithm, which consists in iterative refinement of estimates of parameters P (selected according to a Monte-Carlo or deterministic rule) and the search of the Miller indices mostly close to the experimental d-spacings. The refinement is carried out by the robust Gauss-Newton fitting, and the index assignment by the methods of cluster analysis. A necessary condition for the success of such indexing is the availability of an apriori information about the crystal symmetries and about the maximum volumes and the range of unit cells. Certainly, if the background and useful reflections fully overlap, there is practically no chance for their successful separation. So typical cases, when such a chance exists, are, e.g., if the sizes of unit cells of the background and master crystals don't overlap and, particularly, the background unit cell has a smaller size and higher symmetry than the master one. The same method can be used for the elimination of single spurious reflection.

The method is illustrated by the analysis of a real sample. Models with 2 phases: monoclinic and a tetragonal background, and the 3 phases: monoclinic and two cubic backgrounds, have been used.

s8.m28.o1 **Determination of Composition and strain Field of Nanostructured Semiconductor Materials**. W. Neumann, H. Kirmse, I.Häusler, R. Otto, I. Hähnert *Humboldt University of Berlin, Institute of Physics, Chair of Crystallography, Newtonstrasse 15, D-12489 Berlin, Germany.*

**Keywords: Semiconductors; Quantum Structures; Transmission Electron Microscopy**

Nanostructured semiconductor materials, particularly quantum structures are an important class of materials because the dimensionality on the nanometer scale may drastically change the density of states and the optoelectronic properties. The properties of quantum structures essentially depend on the perfection of their structure, size, arrangement, morphology and chemical composition. For various semiconductor systems of low dimensions including multilayers, islands and quantum dots the potential applicability of transmission electron microscopy (TEM) was demonstrated [1].

Conventional TEM, high-resolution imaging (HRTEM) and digital image analysis were applied to determine strain and chemical composition of nanostructured semiconductor materials. The diffraction contrast method was applied to visualize the strain field in the surrounding of the quantum dots (QDs). For a reliable interpretation of the diffraction contrast features and also of the HRTEM images corresponding image simulations were carried out. Dark-field imaging allows a qualitative analysis of chemical composition using chemically sensitive reflections. Methods of quantitative HRTEM (qHRTEM) were used to measure the local strain and chemical composition on atomic scale. The possibilities and limitations of qHRTEM program packages DALI (Digital Analysis of Lattice Images) [2], CELFA (Composition Evaluation by Lattice Fringe Analysis) [3] and JCPM (Jülich Chemical Mapping Package) [4] will be demonstrated investigating the following systems:

(i) $GaSb_yAs_{1-y}$ QDs on $In_xGa_{1-x}As$ seed grown by metalorganic chemical vapour deposition (MOCVD) on GaAs substrates,

(ii) $Si_{1-x}Ge_x$ islands grown on (001) Si by liquid phase epitaxy (LPE)

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