

**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 i th 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 $S = (d_k)$, $k=1, 2, \dots, m$, 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.