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Making use of coordinate uncertainties in structure comparison

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Keywords: coordinate error estimation, structure correlation, protein structure comparison

The comparison of similar structures is a central step in extracting biological information from structural models. As structural data become available at an ever increasing rate, the set of 'similar structures' to be taken into account for a specific problem can easily contain tens or hundreds of models. For such a situation, the classical approach of pair wise superposition using the root-mean-square-deviation (r.m.s.d.) between superimposed atoms as the central criterion for similarity is clearly inadequate. We suggest to use the fraction of distances that remain identical within experimental uncertainty in an ensemble as a new criterion for structural similarity. We define a conformational similarity index 'C.S.I.' as C.S.I. = n_{id} / n_{all} (where n_{id} and n_{all} are the number of equivalent distances that are identical within error and the total number of equivalent distances, respectively). The C.S.I. can be used (1) to evaluate the overall similarity of groups of structures and (2) as a criterion to find subsets of atoms that are similar within experimental uncertainty. In our current implementation of a C.S.I.-based framework for structure analysis, we use Cruickshank's DPI [1] plus a B-factor based scaling [2] to estimate the coordinate uncertainties of individual atoms. The C.S.I. can be calculated by comparing all CA-CA distances in different models and then used to drive the clustering of models into groups containing models that are identical within error. From these groups, representative models are chosen and analysed further in terms of subsets of atoms leading to a description of a protein in terms of rigid bodies and flexible regions. We demonstrate the approach by analysing the ensemble consisting of crystal structures of protein kinase A as available from the protein data bank. This ensemble contains more than 40 models of the enzyme crystallized in different space groups, with different ligands etc. and shows estimated mean coordinate uncertainties ranging from less than 0.05 Å to more than 0.5 Å. The clustering of the models followed by the analysis in terms of rigid bodies divides the protein into the two known domains and provides an objective basis for optimum superposition and further detailed analysis. A computer program implementing the ideas presented is available from *http://schneider.group.ifom-ieo-campus.it/escet*.

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XRD on nanocrystalline materials - the capability and information content

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Keywords: partial coherence, nanocrystalline composites, X-ray diffraction, local preferred orientation of crystallites

Two years ago, it was shown that adjacent crystallites, which are smaller than approximately 10 nm, can be mutually coherent for X-ray scattering up to relative high diffraction angles if they have sufficient local preferred orientation [1]. Previously, the phenomenon of the (partial) coherence of adjacent crystallites was only known from the theory of the small-angle X-ray scattering [2]. For the wide-angle X-ray scattering, the partial coherence of adjacent crystallites was described via partial overlap of their reciprocal lattice points [1]. Using this theoretical model, it could be shown that the degree of the partial coherence is controlled by broadening of the reciprocal lattice points, which depends on the crystallite size, by the mutual rotation of individual reciprocal lattices, which corresponds to the disorientation of the adjacent crystallites, and by the size of the diffraction vector, because the overlap of the reciprocal lattice points from adjacent crystallites (and thus the degree of the partial coherence) decrease with increasing size of the diffraction vector. From the instrumental point of view, it is needed that the coherence length of X-rays is larger that the distances between the adjacent crystallites [3].
The phenomenon of the partial coherence of adjacent crystallites has already been employed in materials science, particularly in structure research. Primarily, the partial coherence of crystallites was used to determine the true crystallite size in nanocomposite thin films [1, 4] and in nanocrystalline powders [5] with the crystallite size between 10 and 2.5 nm. Furthermore, the high sensitivity of the partial coherence of adjacent crystallites to their local preferred orientation approved the wide-angle XRD to be a suitable tool for a local texture analysis in addition to the standard (global) texture analysis. In nanocomposite thin films, we observed recently that the growth of nanocrystallites with correlated crystallographic orientations favours the formation of inherent lattice strains at the crystallites boundaries separating different crystallographic phases that improves the hardness of these materials. The growth of crystallites with correlated crystallographic orientations can be identified through a high degree of the partial coherence of adjacent crystallites of the same phase. Partial coherence of adjacent nanocrystallites and its influence on the X-ray diffraction line broadening as well as on the materials properties of nanocomposites will be illustrated on the Ti-Al-N, Ti-Al-Si-N and Cr-Al-Si-N systems.

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