

### STRUCTURE AND ELECTRONIC PROPERTIES OF EPITAXIAL Fe-Co-O THIN FILMS

C. L. Chang<sup>1</sup> C. L. Chen<sup>1</sup> C. L. Dong<sup>1</sup> G. Chern<sup>2</sup>

<sup>1</sup>Tamkang University Physics Department 151 Ying-Chuan Rd. TAMSUI 25137 TAIWAN

<sup>2</sup>Department of Physics, National Chung-Cheng University, Chia-Yi, Taiwan, R.O.C.

We report the studies of structure and electronic properties of a series of epitaxial  $\text{Fe}_{1-x}\text{Co}_x\text{O}_y$  ( $0 < x < 1$ ) thin films by x-ray absorption near edge structure (XANES). Our results indicate that for  $x < 0.5$ , the structure is spinel-like, Co occupies not only the octahedral B site but also the tetrahedral A site. For  $x > 0.5$ , the structure changes to rock salt. The average valence of Fe is almost constant. On the other hand, the valence of Co drops from 2.4+ for  $x < 0.5$  to 2+ for  $x > 0.5$ . The cation distribution and their average valence are entirely different from the bulk materials. We propose that the formation of a metastable phase of these Fe-Co-O films is due to the low temperature oxygen plasma assisted MBE growth process.

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**Keywords:** METAL OXIDE XANES CATION DISTRIBUTION

### POLYMORPH SELECTION, AND CRYSTAL PREDICTION AS PART OF CRYSTAL ENGINEERING STRATEGY

N. Blagden<sup>1</sup> R Davey<sup>2</sup> W Cross<sup>2</sup>

<sup>1</sup>University of Bradford School of Pharmacy Richmond Building BRADFORD WEST YORKSHIRE BD7 1DP UK <sup>2</sup>Department of Chemical Engineering UMIST Manchester M60 1QD UK

Can crystal prediction be used as part of an integrated strategy of crystal engineering strategy is the focus of our current work. For crystal engineering to achieve its goal of being able to select a specific molecular assembly based on synthon stereochemistry, the self-assembly of other viable assemblies would need to be discouraged. The implication of this observation is that crystal structure prediction and polymorph selection procedures must also be included into a crystal engineering strategy. The work in my talk will cover our experiences to date in using crystal structure prediction to explore possible modes of assembly of 2-amino-4-nitrophenol (ANP) molecules in the solid state. The results from this simulation were employed for the rational selection of solvents for the isolation of the solid phase by solution crystallisation. How an understanding of polymorph selection and crystal structure prediction may be used in crystal engineering for this type of situation will be examined.

**Keywords:** CRYSTAL PREDICTION ENGINEERING

### QUADRATIC APPROXIMATION OF THE MAXIMUM-LIKELIHOOD CRITERION

P. Afonine<sup>1,2</sup> V. Y. Lunin<sup>1,3</sup> A. Urzhumtsev<sup>1</sup>

<sup>1</sup>LCM3B Universite Henri Poincare, Nancy I Faculte Des Sciences B.P. 239, UHP NANCY 54506 FRANCE <sup>2</sup>Centre Charles Hermite, Nancy <sup>3</sup>IMPB, Pushchino

One of major defaults of the traditional least-squares (LS) refinement is that in the case of incomplete model the existing atoms are refined to incorrect positions. Maximum likelihood (ML) criterion allows us to essentially reduce this effect. The approximation of the maximum likelihood criterion by a quadratic functional allows us to understand the features of the ML refinement and its advantages with respect to the traditional least-squares refinement. This approximation corresponds to the LS criterion calculated with Fobs substituted for some modified  $F^*$  values (Afonine et al., 2001; Lunin et al., 2002) and weighted respectively by  $w^*$ . These  $F^*$  and  $w^*$  are calculated using some probability distribution parameters  $\alpha / \beta$  obtained through the ML approach. Such approach gives the results of the same quality as the ML realized for example in CNS and much better than the results obtained by LS. Even more, such approximation done with a modified estimation for  $\alpha / \beta$  allows to essentially improve the convergence of the refinement with such criterion, and obtain the results much better than previously. This procedure does not need a special programming and can be realized in any LS refinement suite.

References

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**Keywords:** MAXIMUM LIKELIHOOD, LEAST-SQUARES, ATOMIC REFINEMENT

### CRYSTAL STRUCTURE PREDICTIONS IN ASSISTANCE TO EXPERIMENTAL STUDIES OF SOLID-STATE PHENOMENA AND PROCESSES

A. Dzyabchenko

Karpov Institute of Physical Chemistry 10 Vorontsovo Pole MOSCOW 103064 RUSSIA

Since the pioneering work of Kitaigorodskii in the beginning of the sixties of the last century, the idea of *ab initio* crystal structure prediction has long been regarded as solely an academic problem rather than that of practical importance. Nowadays, it gains still growing interest from experimentalists seeking the understanding of their observations of the solid-state phenomena and processes at a detailed structural level. This poster presents our methodology and tools for organic crystal structure prediction. Program PMC serves for global minimization of lattice energy. Program PMCDAT makes the preparation of input data to PMC an easy procedure; it contains also facilities to transform the rigid-body structure descriptions under changing the unit-cell setting. Program CRYCOM of crystal structure comparison is capable to reveal the similarity of structures, to determine the shortest paths connecting the polymorphic structures and to reconstitute the space-group symmetry of a structure. Their use will be illustrated with examples of successful structure predictions for a high-pressure phase of benzene, a metastable phase of piracetam, and the pressure-polymerized fullerenes  $\text{C}_{60}$  and  $\text{C}_{70}$ . Supported by Russian Foundation for Basic Research (95-03-09418, 99-03-32962 and 02-03-32951).

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