We present a method to improve the electron density for missing atoms of macromolecular structures, using Likelihood maximization [1,2,4] with entropy loss constraints [1,2]. Both the model for the structure factor offset $F_0$ and the one for its associated uncertainty can incorporate: 1. a partial structure factor offset $F_{h}$, the latter are varied to increase likelihood, while keeping the entropy of $q(x)$ relative to $m(x)$ at a constrained maximum. The log-likelihood gain for the free-set reflections is monitored to validate the extra detail introduced in $q(x)$. The method has aided the completion of two macromolecular complexes starting from Molecular Replacement phases [5,6].

References:
5. Ng et al. (2000) Nat. Struct. Biol. 7(8), 653-657
6. Hanzl-Bayer et al. (2000) EMBO J. accepted for publication

Keywords: MAXIMUM LIKELIHOOD MAXIMUM ENTROPY DENSITY MODIFICATION

Low-temperature HREM analysis of charge- and orbital-ordered structures in perovskites

Y. Matsu’i1, T. Nagai1, T. Asaka1, K. Kimoto1, T. Kimura1, Y. Tokura1
1Advanced Materials Laboratory National Institute for Materials Science 1-1 Namiki TSUKUBA IBARAKI 305-0044 JAPAN 2Department of Applied Physics, University of Tokyo

Charge-orbital ordered structures have intensively been investigated by low-temperature electron diffractometry and low-temperature HREM, due to their close relation to characteristic electro-magnetic properties such as colossal magneto-resistance (CMR) in manganites. Recently, superstructure models including sinusoidal lattice distortions have been proposed for commensurately doped layered-perovskites, Nd$_{x}$Sr$_{x}$MnO$_{3}$ $(x = 2/3, 3/4)$, where, we present our recent data of HREM investigation of Nd$_{0.5}$Ca$_{0.5}$MnO$_{3}$ which show charge-orbital ordering at low temperature, not only in commensurate but also in incommensurate doping levels $(0.55 < x < 0.75)$. Polycrystalline samples of Nd$_{0.5}$Ca$_{0.5}$MnO$_{3}$ were prepared by the standard ceramic method. The HREM observation was conducted for crushed and ion-milled specimen, by a Hitachi HRTEM images. Low-temperature electron diffraction measurements revealed the formation of superstructures accompanied by charge-orbital ordering transition in the composition range of $0.55 < x < 0.75$. The wave vector of structural modulation in the system can be derived as $k_\text{S} = (1-x) a^*$. The low-temperature HREM images, taken at 80K, show long-period superlattice fringes and sinusoidal transverse modulation of the crystal structure, with the period of $a/(1-x)$, i.e. 3a for $x = 0.67$. Such sinusoidal modulations are in good agreement with absence of higher-order superlattice reflections in electron diffraction patterns. Also, effects of double-reflection should be taken into account for detailed interpretation of HREM images.

References

Keywords: HREM LOW-TEMPERATURE CHARGE-ORDERING