function. In the conventional approach a just significant 3rd order parameter was determined but the existence of fourth order parameters could not be conclusively established because of very high correlation between second and fourth order parameters of the least squares refinement model.
For comparison with results of the conventional treatment, parameters for the anharmonic vibrations have been derived by a 3-dimensional fit of a One Particle Potential model to the MEM nuclear density. Significant values for the cubic term, α_{33}=-0.340(5)eV/A^3 and a quartic term, β_{20}=9.89(1)eV/A^4 were found. Maps of the calculated nuclear densities for the assumed model with the above mentioned parameters are shown in Fig.2. In this study it was found that comparison between maps of the MEM nuclear density and maps calculated based on an assumed potential model provided an effective help in determining which model is the most appropriate model for describing the intrinsic anharmonic effects on the nuclear density distribution in Be metal.

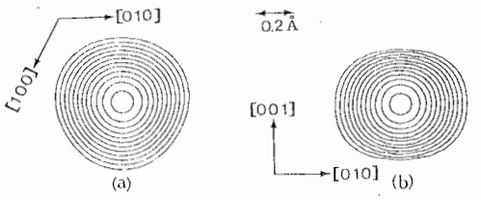

Fig.1 MEM nuclear densities of (a) basal plane and (b)(100).

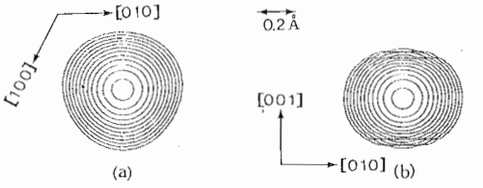

Fig.2 The calculated nuclear density of (a) basal plane and (b) (100).

PS-02.03.10 MAXIMUM ENTROPY METHOD ANALYSIS OF X-RAY AND NEUTRON POWDER DIFFRACTION DATA OF ANATASE.
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In X-ray diffraction, X-ray photons are scattered by electrons in materials, while neutron beams are diffracted by nuclei when there is no magnetic interactions. It is, therefore, appropriated to try to reconstract the electron and nuclear density distribution of the crystalline materials from X-ray and neutron diffraction data, respectively. There have been, however, not known how to restore such electron and/or nuclear density distribution directly from the observed structure factors by diffraction without using any structural model. Recently Sakata & Sato (Acta Cryst., 1990, **A46**, 263-270) has successfully applied the Maximum Entropy Method (MEM) to restore the precise electron density distribution from the accurately determined structure factors. Following to them, it was shown that the accurately measured powder data were suitable for the MEM analysis.

The success of the method depends on the fact that the electron density is always positive. In order to analyse neutron diffraction data by the MEM, it is necessary to overcome the difficulty of negative scattering length for some atoms, such as H, Ti and Mn. In order to overcome the difficulty, Sakata, Uno, Takata & Howard (J. Appl. Cryst., 1993, **26**, in press) has proposed a new method, which deal with, not scattering length densities, but nuclear densities which are always positive. The new method was successfully applied to a rutile (TiO_2) case. This is, however, only one example of the new method. In this paper, the results of MEM analysis for anatase will be given. The data set used in the analysis are collected by powder diffraction experiments for both X-ray and neutron cases.

The MEM maps of anatase are shown in Fig. 1 (a) for electron density and (b) for nuclear density distributions, respectively. In Fig. 1 (a), the chemical bonding state of anatase is very well depicted, which are two kinds of covalant bonding between Ti and O atoms. On the other hand, the nuclear densities in Fig. 1 (b) are simple features of smearing by thermal vibrations. These general features of MEM maps for electron and nuclear densities are very reasonable from physical view point and the present example again proves the usefulness of MEM analysis in crystallography when it is applied to powder diffraction data.

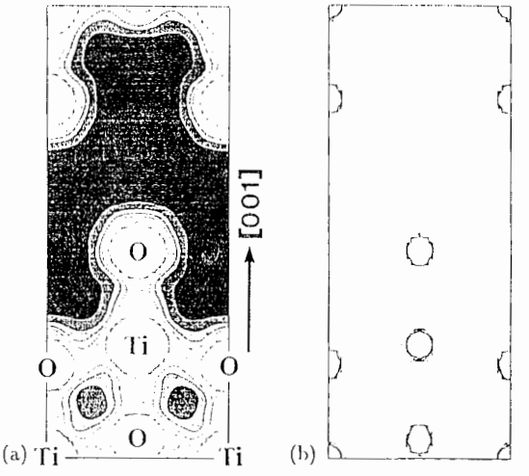

Fig. 1 The MEM maps of anatase (100) plane for (a) electron densities and (b) nuclear densities obtained from powder diffraction data. Contour lines are 0.2 intervals up tp 2.0 e/Å^3 in (a) and 0.1 intervals up to 1.0 x10^{-12} n/Å^3 in (b).

02.04 – Direct Phasing from Electron Diffraction Data for Crystal Structure Analysis

MS-02.04.01 DIRECT PHASING IN ELECTRON CRYSTALLOGRAPHY. By D. L. Dorset* and M. P. McCourt, Electron Diffraction Department, Medical Foundation of Buffalo, Inc., 73 High Street, Buffalo, NY 14203 USA

Although the concept of using electron diffraction intensity data for *ab initio* structure analyses was conceived by B. K. Vainshtein, Z. G. Pinsker and their co-workers, acceptance of these data for quantitative determinations is anything but widespread. Recently, the application of traditional direct phasing methods used in X-ray crystallography to electron crystallography, by themselves or in combination with independent phase information from electron microscope images, has shown overwhelmingly that the earlier effort in Moscow was generally correct. Successful analyses have been carried out for small organic compounds, paraffins and their derivatives, linear polymers, larger aromatics with heavier atoms, and even a number of inorganic compounds, either using data collected in the original studies or newer data collected at higher

