14. ELECTRON DIFFRACTION AND ELECTRON MICROSCOPY

14.2-1 THE APPLICATION OF THE MULTISLICE METHOD TO THE CALCULATION OF CONVERGENT BEAM RHEED PATTERNS. By A.L. Smith, Department of Physics, Monash University, Clayton, Victoria 3168, Australia and D.F. Lynch, CSIRO Division of Materials Science and Technology, Noramby Road, Clayton, Victoria 3168, Australia.

A computational scheme is outlined for the calculation of high energy electron dynamical diffraction patterns in the Bragg, i.e. reflection geometry, case. The influence of the boundary conditions is shown to be quite different from the more widely studied Laue, i.e. transmission geometry, case.

Results of this scheme are in particular shown to enable a detailed understanding of convergent beam (CR) RHEED patterns and their possible application to surface characterisation.

The scheme used is an adaption of UED methods, and thus deals well with the tangency condition of the reciprocal lattice rods to the Ewald sphere. However, it may be possible to shorten the present scheme as it provides a rather complete description of backscattering, a weak process at high energies.

14.3-1 GEOMETRIES AND LARGE-AMPLITUDE MOTIONS OF MOLECULES STUDIED BY A COMBINED ANALYSIS OF GAS ELECTRON DIFFRACTION, SPECTROSCOPY AND AB INITIO CALCULATION. By T. Egawa, Y. Ohshima, K. Kuchitsu, S. Yamamoto, N. Nakata, T. Hamada and Y. Kuchitsu, Department of Chemistry, Faculty of Science, The University of Tokyo, Bunkyo-ku, Tokyo 113, Japan.


(1) Structures of conformers: Ethylamine and 1,2-diaminohydrazine. The structures of the gauche (g) and trans (t) conformers of CH3CH2NH2 were determined by a joint analysis of the GED intensity, the rotational constants, and an ab initio calculation using a 6-31G** basis set. The C-N-C dihedral angle for g = 4.0(6)° and 165.3(18)° for 20 and 00, respectively, and the enthalpy difference, DH(00-20), was 0.2(8) kJ/mol (K. Kuchitsu et al., J. Phys. Chem., 1987, 91, in press).

(2) Large-amplitude motions in cyclobutane and carbon suboxide. The GED intensity for (CH2)4, was analysed jointly with the rotational constant determined by an FTIR spectrum. The ring dihedral angle, 0, and the CH2-rocking angle, δ, were found to be 27.9(15)° and 6.2(12)°, respectively, the CH2 groups being rocked toward each other. The coupling between the puckering and rocking modes has a strong influence on the estimation of the effective mass for the puckering motion, and only by inclusion of this coupling was it possible to make the spectroscopic data fully consistent with the GED data (T. Egawa et al., J. Chem. Phys., submitted for publication).

The geometrical structure and the potential function for the large-amplitude ω (C≡C bending) mode for C≡C≡C≡C were determined by a joint analysis of the GED intensity, the intervals of the ω levels, and the rotational constants. The C≡C bond length and the C≡C angle were found to change with the ω level; the C≡C bond is stretched and the C≡C angle is bent slightly in the same direction when the C≡C angle is bent. The potential function has a barrier of 27(3) cm⁻¹ and a minimum at [C≡C≡C=160.2(6)°]. The ω and C≡C distances were determined to be 1.2761(15) Å and 1.1602(15) Å, respectively (Y. Ohshima et al., to be published).

14.4-1 STRUCTURE REFINEMENT FROM HREM IMAGES USING DIRECT DIFFERENCE METHODS. P. Goodman, Division of Materials Science and Technology, CSIRO, Clayton, Vic. 3168, Australia, S. Rae, Dept. of Physics, Monash University, Clayton, Vic. 3168, Australia, and F. Tulloch, Division of Protein Chemistry, CSIRO, Parkville, Vic. 3052, Australia.

In the past, comparisons of experimental high resolution images from inorganic compounds have been compared with those obtained by N-visual matching. The agreement obtained in order to decide upon a model structure has been qualitative only.

One class of structures has proved extremely difficult to match in this way, from modifications to the x-ray determined structure, assuming neutral spherical atoms. These are oxides with large, partially filled tunnels. The present paper describes an attempt to refine the local structure of a tunnel site in Rb2Sb2O7 using a digitised image. (obs. - calc.) can be inverted for a particular defocus to give an approximate V(z,y) value, leading to a refinement cycle.

The search for a converging cycle leads to a close scrutiny of invertible approximations to the N-beam image.