14.2-1   THE APPLICATION OF THE MULTISLICE METHOD TO THE CALCULATION OF CONVERGENT BEAM RHEED PATTERNS. By A.E. Smith, Department of Physics, Monash University, Clayton, Victoria 3168, Australia and D.F. Lynch, CSIRO Division of Materials Science and Technology, Normanby 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 (CB) RHEED patterns and their possible application to surface characterisation.

The scheme used is an adaption of LEED 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. Yamanouchi, S. Yamamoto, M. Nakata, Y. Hamada and K. Kuchitsu, Department of Chemistry, Faculty of Science, The University of Tokyo, Bunkyo-ku, Tokyo 113, Japan.

Information on the geometries and potential functions for free molecules provided by the intensity of gas electron diffraction (GED) was analyzed with the aid of data obtained from other experimental and theoretical sources such as microwave and infrared spectroscopy and ab initio calculation. The method of analysis has been discussed in recent review articles (K. Kuchitsu, Fifty Years of Electron Diffraction, Edited by P. Goodman, International Union of Crystallography, Reidal, Dordrect, Part III, Chap. 3, 1981, 356-377. K. Kuchitsu, Methods and Applications in Crystallographic Computing, Edited by S. R. Hall and T. Ashida, 1984, 441-449, Oxford: Clarendon Press. K. Kuchitsu et al., Stereochemical Applications of Gas-Phase Electron Diffraction, Edited by I. Hargittai, The Series: Methods in Stereochemical Analysis, Edited by A. P. Marchand, 1987, Florida: VCH Publishers Inc., in press). The merits and limitations of this method applied to molecules with large-amplitude motions are discussed in comparison with those of the crystallographic methods for structure analysis by taking a few examples.
(1) Structures of conformers: Ethylamine and 1,2-dimethylhydrazine. The structures of the gauche (g) and trans (t) comformers of $CH_3CH_2NH_2$ were determined by a joint analysis of the GED intensity, the rotational constants, and the optimized geometries estimated by a $4-31G(N^*)$ basis set. The C-C-N angles were determined separately for the g and t conformers, 109.7(3) and 115.0(3)°, respectively, and the enthalpy difference, $\Delta H(g-t)$, was estimated to be 1.3(8) kJ/mol (Y. Hamada et

al., J. Mol. Struct. 1986, 146, 253). The structures of the inner-outer (IO) and outer-outer (OO) conformers of $CH_3NHNHCH_3$ were determined by a joint analysis of the GED intensity, the rotational constants, and an ab initio calculation using a $4-31G(N^*)$ basis set. The C-N-N-C dihedral angles were 87.8(7) and 165.3(18)° for IO and OO, respectively, and the enthalpy difference, $\Delta H(OO-IO)$, was 0.2(8) kJ/mol (K. Yamanouchi et al., J. Phys. Chem., 1987, 91, in press).
(2) Large-amplitude motions in cyclobutane and carbon suboxide. The GED intensity for $(CH_2)_4$ was analyzed jointly with the rotational constant determined by an FTIR spectrum. The ring dihedral angle, θ, and the CH_2-rocking angle, β, were found to be 27.9(16) and 6.2(12)°, respectively, the CH_2 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 ν_7 (C=C=C bending) mode for O=C=C=C=O were determined by a joint analysis of the GED intensity, the intervals of the ν_7 levels, and the rotational constants. The C=C bond length and the C=C=O angle were found to change with the ν_7 motion; the C=C bond is stretched and the C=C=O angle is bent slightly in the same direction when the C=C=C angle is bent. The potential function has a barrier of 27(5) cm^{-1} and a minimum at $\angle C=C=C = 160.2(4)°$. The C=C and C=O distances were determined to be 1.2761(15) 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 P. 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 $Rb_{22-5x}Nb_{54+x}O_{146}$ using a digitised image. $(I_{obs} - I_{calc})$ can be inverted for a particular defocus to give an approximate $V(x,y)$ 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.