14.1-01   A UNIFIED DERIVATION FOR SMALL ANGLE ELASTIC SCATTERING OF HIGH ENERGY ELECTRONS. By R. Portier and D. Gratias[†], C.E.C.M./CNRS, 15 rue G. Urbain, 94400-Vitry, FRANCE ([†] Present address: Department of Materials Science & Mineral Engineering, University of California, Berkeley, CA 94720, USA.)

Numerous methods have been derived for the calculation of dynamical elastic scattering of high energy electrons in a crystal. Although these methods often take quite different forms they all lead to similar results. The present investigation proposes a unified derivation which shows that usual methods correspond to different, but equivalent, ways of solving the fundamental equation (1) numerically. The basic point is that the small angle scattering approximation leads to a time-dependent like Schrödinger equation and therefore to an evolution operator $U(t,t_o)$ solution of

$$(1) \quad i\frac{\partial}{\partial t}U(t,t_o) = (H° + V(t))\, U(t,t_o)$$

where t represents the coordinate along the propagation direction. If the potential $V(t)$ may be considered as constant along the propagation direction, then the solution of (1) is simply

$$U(t,t_o) = \exp\,[-i(H° + V)(t-t_o)]$$

which is the usual scattering matrix expression. If $H° \ll V$, then $U(t,t_o)$ has the form

$$U(t,t_o) \simeq \exp\,[-i\int_{t_o}^{t} V(\tau)d\tau],$$

corresponding to the phase grating approximation. If V is not independent of t, the U may be expanded in a time dependent perturbation series corresponding to the diffraction optic approach, etc. This unified approach, based on a quantum mechanical formulation is a convenient method for describing small angle elastic scattering, and leads to possibly new techniques for approximate calculations.

14.1-02   DIFFRACTION CONTRAST RETAINED BY INELASTICALLY SCATTERED FAST ELECTRONS. By C.J. Rossouw and M.J. Whelan, Department of Metallurgy & Science of Materials, University of Oxford, U.K.

A theory for phonon scattering of fast electrons (Rez, Humphreys and Whelan, Phil. Mag. 35 (1977) 81) has been developed to predict the plasmon and K-loss distribution of 80kV electrons in diffraction patterns formed from single crystals. The formation of Kikuchi lines from these different electronic excitations is demonstrated. The results have implications for the microanalysis of light elements in crystalline materials by electron energy loss techniques. Here the ratio of the low energy loss to characteristic energy loss intensity is used together with the relevant cross-section to predict the number of atoms giving rise to the characteristic loss. Energy loss analysis based on the theory of characteristic losses from single atoms may yield inaccurate results due to the non-symmetrical angular distribution of electrons scattered with energy loss in crystals. Errors may be compounded under diffraction conditions where the elastic beam displays strong extinction since finite apertures in the diffraction plane will still allow a considerable loss signal to be recorded (Rossouw and Whelan, to be published in Ultramicroscopy). Calculations which show varying diffraction contrast in the plasmon loss beam when an aperture is displaced in different directions from diffracted beams are in good agreement with experiment. In weak-beam techniques, inelastic scattering from neighbouring beams in a systematic row will raise background but not interfere with diffraction contrast.

14.1-03   POINT GROUP DETERMINATION FROM SYMMETRICAL MANY-BEAM CBED PATTERNS. By M. Tanaka and R. Saito, Physics Department, Faculty of Science, Tohoku University, 980 Sendai, Japan.

The point group determination from CBED patterns developed by Buxton et al. (Philos. Trans. R. Soc. London A, (1976) 281 171) is based on the symmetries appearing in the zone axis pattern and patterns taken at the Bragg settings of +G and -G reflections. Tinnappel (Ph. D. Thesis, Technical Univ., Berlin, 1975) considered the symmetries appearing in the symmetrical many-beam (SMB) CBED patterns, in contrast with Buxton et al. who considered the two-beam case. It is worth-while making clear systematically the relations between symmetries appearing in SMB patterns and the diffraction groups. The relations can be derived by the graphical method for all diffraction groups. However, five groups 1, 1_R, 2, 2_R and 21_R are left out of consideration, since the possible three-beam excitation in these groups gives no more information than the two-beam case of Buxton. As an example, the symmetry table of the pattern and its illustration for the diffraction group $6m_Rm_R$ is shown here. The zone-axis pattern is rather suitable for finding the two-dimensional symmetry elements. The SMB pattern is useful for finding simultaneously plural number of the three-dimensional symmetry elements. The two-dimensional rotational symmetry elements exhibit their characteristic rather in a pair of SMB patterns taken at different Bragg settings. In SMB method the existence of the inversion center can be found from one photograph, and many diffraction groups can be determined from one photograph, whereas two or three photographs are required in Buxton's theory. For example the diffraction groups having 4-fold axis are distinguished from each other from a SMB photograph, whereas two photographs are necessary for distinguishing the pairs (4, 41_R) and (4mm, $4mm1_R$) by Buxton's method. By using the present method originated with Tinnappel together with Buxton's method, the point group determination can be carried out more easily and quickly.
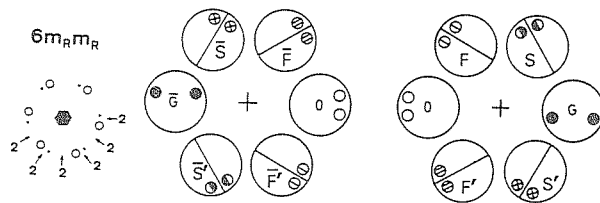
diffraction group $6m_Rm_R$

	G	m_2		±G	$2m_R(m_2)$
	O	m_2	two sets of	±O	$2m_2(m_2)$
symmetrical	F	m_2	symmetrical	±F	1
six beam	S	m_2	six beam	±S	1
pattern			pattern		
	FF´	1		F´F̄	$2m_R(m_2)$
	SS´	1		S´S̄	$2m_R(m_2)$