

2. RECIPROCAL SPACE IN CRYSTAL-STRUCTURE DETERMINATION

least-squares refinement of diketopiperazine (Dorset & McCourt, 1994a). It is obvious that, if a global minimum is sought for the crystallographic residual, then dynamical structure factors, rather than kinematical values, should be compared to the observed values (Dorset *et al.*, 1992). Ways of integrating such calculations into the refinement process have been suggested (Sha *et al.*, 1993). Otherwise one must constrain the refinement to chemically reasonable bonding geometry in a search for a local *R*-factor minimum.

Corrections for such deviations from the kinematical approximation are complicated by the presence of other possible data perturbations, especially if microareas are being sampled, *e.g.* in typical selected-area diffraction experiments. Significant complications can arise from the diffraction incoherence observed from elastically deformed crystals (Cowley, 1961) as well as secondary scattering (Cowley *et al.*, 1951). These complications were also considered for the larger (*e.g.* millimetre diameter) areas sampled in an electron-diffraction camera when recording texture diffraction patterns (Turner & Cowley, 1969), but, because of the crystallite distributions, it is sometimes found that the two-beam dynamical approximation is useful (accounting for a number of successful structure analyses carried out in Moscow).

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