written (in Fortran) to be easily portable to other computer platforms. This program has begun to play a major role in our studies by providing a tool which measured diffraction data can be compared to 3D computer simulations. The wide applicability of this program will be demonstrated by showing example diffraction patterns from simulated size-effect displacements in metallic alloys, mineral systems exhibiting oxygen vacancy order and cation relaxations, and conformational disorder in organic crystals. The program and a manual describing its use will be made freely available.

MS-02.05.03 DIFFUSE SCATTERING AND INTRA-MOLECULAR FLEXIBILITY IN PROTEINS by J.-P. Benoit, P. Faure and J. Doucet, LURE et Laboratoire de Physique des Solides, Universite Paris-Sud, F91405 Orsay, France

The growing interest in the dynamical behaviour of proteins is motivated by the fact that in many cases the functional roles of these biological molecules do not only depend on their rigid three-dimensional structure but also on their deformability or flexibility. The loss of function in proteins is often accompanied by the occurrence of ordered conformational changes that can be detected by X-ray diffraction. In the macromolecular framework, the large range in displacements of atoms results in a large range of protein dynamics.

MS-02.05.04 STUDIES OF DIFFUSE SCATTERING REVEAL LIQUID-LIKE DISORDER IN PROTEIN CRYSTALS by Y. Li, D.L.D. Caspar, B. Yu, Rosenstiel Basic Medical Sciences Research Center, Brandeis University, Waltham, MA 02254-9110, U.S.A., and J.B. Clarage, Department of Biochemistry and Celi Biology, Rice University, Houston, TX 77251.

Diffuse scattering from protein crystal, notably haloes surrounding Bragg reflections, contain information about both the amplitude and correlation of atomic movements in the protein molecules. We have developed an analytical model for simulating diffuse scattering from protein crystals by representing the average Patterson function as the convolution of the peaks in the ideally ordered Patterson with a Gaussian whose variance is a function of the mean-square atomic displacement and a correlation function which describes coupling between movements. Based on this model we have simulated diffuse scattering data collected from lysozyme and insulin crystals in terms of an exponentially decaying correlation function which has two components separating short-range and long-range coupling. The results show that the coupling of atomic movements in these highly ordered protein crystals is mostly short-ranged, similar to that in liquid rather than that in elastic solids. The total mean square atomic displacements for tetragonal lysozyme, triclinic lysozyme and Zn tomonohedral insulin arc 0.25 Å², 0.15 Å², and 0.2 Å², respectively. About 90% of the total mean square displacements in these crystals are correlated over distances the size of one amino acid residue (~ 6 Å). Movements that are correlated over the distance the size of the protein molecule (~ 50 Å) account for about 5% of the total displacements. Experiments are under way to measure diffuse scattering data from cubic insulin crystals at different pH and ionic strength, and to analyze these data in terms of the analytical model described above and empirical models about switching between conformational substates that are evident at high resolution structures.

MS-02.05.05 MODELS FOR DIFFUSE SCATTERING FROM PROTEIN CRYSTALS by Nobuhiko Go, Kenji Mizuguchi and Akinori Kidera, Department of Chemistry, Faculty of Science, Kyoto University, Saky-ku, Kyoto 606, Japan, and Protein Engineering Research Institute, 6-3-3 Furusato, Saka, Osaka 565, Japan

We have developed a new theoretical framework for the study of X-ray diffuse scattering from protein crystals, in which we start from a general equation and introduce a series of approximate models, appropriate for analyses of experimental data obtainable with different degrees of precision. When a high precision data are available, we can employ essentially the same model developed for the recently developed method, NPMREF (Kibrick, A.A. et al., 1992) (NPMREF) of refinement of protein structure from the usual Bragg diffraction. Further approximation is based on the assumption that the covariance matrix of atomic displacements can be expressed by using a relatively simple empirical correlation function. The formalism using the correlation matrix retains information about atomic details and allows us to introduce a variety of models, in which (1) the effect of higher order scattering is included, (2) intra-and intermolecular correlations can be distinguished, and (3) amplitudes of fluctuations can be distinct from the usual refinement of protein structure from the usual Bragg diffraction. Further approximation is based on the assumption that the covariance matrix of atomic displacements can be expressed by using a relatively simple empirical correlation function. The formalism using the correlation matrix retains information about atomic details and allows us to introduce a variety of models, in which (1) the effect of higher order scattering is included, (2) intra-and intermolecular correlations can be distinguished, and (3) amplitudes of fluctuations can be

MS-02.05.06 DIFFUSE SCATTERING IN ELECTRON DIFFRACTION FROM MOLECULAR ORGANIC-AND PROTEIN-CRYSTALS; ANALYSIS OF CRYSTAL-CRYSTAL PHASE TRANSITIONS. By Douglas L. Dorsett, Electron Diffraction Dept., Medical Dtrm. of Buffalo, Inc., 73 High St., Buffalo, NY 14203 USA

Electron diffraction patterns from molecular organic crystals often contain a pronounced directed diffuse component