dimensional graphic structure display is also implemented for organic substances. All search criteria can be integrated with Boolean operators, including AND, OR and NOT, providing considerable flexibility in searches. For example, the user can search for substances containing only elements "Si" AND "O"; the user can also search for all substances containing "Si" OR "O".

The PCPDFWIN program has been developed as a Microsoft Windows 3.1 application. It runs on an Intel 386 (or above) based computer and requires at least 4 MB RAM, 6 MB hard disk space, a mouse, Microsoft Extensions and a PDF2 database on CD-ROM.

based on the coincidence site lattice concept and a modified theoretico-numerical algorithm (Santoro A., Mighell A.D., Acta Crystallogr., 1973, A29, 169-175); an analysis of structure defects connected with the symmetry aspects of genetic relations between the substrate and layer structures; computer graphics for visualization of the interfacial region.

The data base contains the following information: crystal-geometrical parameters: structure type and unit-cell constants; dependence of these parameters on temperature including the temperatures and types of phase transformations; dielectric constants; peculiarities of phase diagrams; data source.

PS-18.01.09 SEQUENCE DEPENDENCE OF NON-PLANARITY OF PEPTIDES, AND EFFECT ON SECONDARY STRUCTURES. By N. Sukumar and Vasantha Pattabhi*, Department of Crystallography and Biophysics, University of Madras, Madras 600 025, India.

Non-planarity of peptides has been predicted from quantum chemical theory, and has also been observed frequently in crystal structures. A systematic study of this phenomenon is expected to give informations on the flexibility of peptide plane, and also help in model-building studies.

Class 48 of the Cambridge Crystallographic Data Base has been surveyed with this aim in mind. The analysis shows that deviations from planarity $(\Delta\omega)$ range from $0°$ to $20°$ depending on the sequence. In general, deviations for Ser, Asn, Lys and His are very low in contrast with those for Phe, Pro and Leu. If Gly precedes or succeeds any residue, the deviation from planarity is significant. A linear correlation between molecular weight and torsion angle ω has been observed, indicating that deviations from planarity are involved to avoid steric interactions, and in some cases to enable hydrogen-bond formation. The analysis was extended to study the correlation between $\Delta\omega$ and the secondary structural features. The following observations have been made from the study. (i) The direction of the deviation, and the handedness of the helix seem to be correlated. (ii) In the case of peptides adopting bent conformation, the $\Delta\omega$ values are uniformly small. (iii) No such correlation was seen in the case of extended structures.

PS-18.01.10   COMPUTER-AIDED DESIGN OF NON-ISOMORPHIC HETEROCOMPOSITIONS. By A.N. Efimov, A.O. Lebedev*, Ioffe Physical-Technical Institute, St. Petersburg, Russia.

The correct choice of substrate compound and of its crystallographic orientation is of great importance for epitaxial growth of HTS. The following conditions concerning the substrate must be verified: compatibility of the substrate material with the physico-chemical conditions of growth and subsequent processing; absence of chemical interaction between substrate material and HTS; geometrical match with HTS-structure as a prerequisite for creating perfect single crystalline epitaxial layers (taking into account the temperature dependence of lattice parameters); physical properties needed for the concrete device application (for instance the small dielectric loss for HF- and UHF-range); low cost of starting materials and possibilities for industrial manufacturing of substrates. The optimal design of heterocompositions is nearly impossible without computers due to the number of compounds, and due to the number of requirements to be taken into account. The present computer-aided design package for heterocompositions includes the following program units: an analysis of metric match

PS-18.01.11 A UNIVERSAL FILE FORMAT FOR POWDER DIFFRACTION DATA ARCHIVE AND INTERCHANGE: THE IUCR CRYSTALLOGRAPHIC INFORMATION FILE FORMAT. By B.H. Toby, Air Products & Chemicals Inc., 7201 Hamilton Blvd, Allentown, PA 18195, USA, J.I. Langford*, School of Physics & Space Research, University of Birmingham, Birmingham B15 2TT, UK and S.R. Hall, Crystallography Centre, University of WA, Nedlands 6009, Australia.

Powder diffraction data definitions have been devised for use with the Crystallographic Information File (CIF) facility for data storage and exchange. These will permit the ready exchange of raw and processed powder data generated by diffractometers of every type – commercial sealed-tube X-ray instruments, single-wavelength synchrotron and neutron systems and energy-dispersive or time-of-flight experiments.

CIF has been developed by the IUCr for the storage of crystallographic data which range from measured intensities to structural diagrams and text in a form suitable for publication (Hall et al., Acta Cryst. A47, 655-685). CIF is composed of ASCII characters which may be edited in the normal way or transmitted via international networks (eg E-mail or FTP). A CIF is completely self-descriptive, in that data items are identified by unique tags, known as data names, which may be defined locally or globally. Global data items (ie those used outside the local environment) are carefully defined in a CIF data-name directory that is also stored electronically in a CIF-like format.

Powder diffraction data are usually measured by means of a computer-controlled diffractometer, or obtained from film by a densitometer, and are stored in a data-file format specific to the instrument used. Typically, these data are then processed by using computer programs modified to use data with the local format. If the data are to be published or archived, the diffraction pattern will often be reduced to a table of peak position and intensity values. Apart from the requirement to standardise the data-processing software, the need for a global exchange of unprocessed powder diffraction data is increasing. This need arises because of the use of total-pattern methods for

(1) crystalline phase identification and quantification,

(2) ab initio structure determination,

(3) structure refinement,

(4) studies of microstructure and

(5) characterisation of materials with limited ordering (eg polymers and clays, where the diffraction pattern cannot adequately be represented by a set of peak parameters).