The algorithm developed by Porter (1978) for shading spheres to be darkened near their peripheries also computes the proper appearance of the line of intersection of two spheres wherever interpenetration occurs, in contrast to some simpler systems which draw a complete disc for whichever sphere is forward of the other. Provided that all opaque spheres are drawn first, the system is also capable of representing transparent spheres by darkening the colour of the existing background inside, and especially near the edge of, discs representing transparent foreground spheres.

Other systems that produce space-filling pictures of a similar general character have been produced by Motherwell (1978), by Sundaram & Radhakrishnan (1979) and by Lesk (next section).

3.3.3.1.3. *Lesk & Hardman software*

The complexity of macromolecules is a formidable obstacle to perceiving the basic features of their construction and the stylized drawings produced by this software following the artistry of Richardson (1977, 1981, 1985) enables the internal organization of such molecules to be appreciated readily. The software is capable of mixing several styles of representation, among them the Richardson style of cylinders for α-helices, arrows for β-strands and ribbons for less-organized regions, or the creased-ribbon technique for the whole chain, or a ball-and-stick representation of atoms and bonds, or space-filling spheres. All these styles are available simultaneously in a single picture with depth cueing, colour and shading, and hidden-feature suppression as appropriate. It is also able to show a stylized drawing of a complete molecule together with a magnified part of it in a more detailed style. See Lesk & Hardman (1982, 1985).

3.3.3.1.4. *GRAMPS*

This system, due to O'Donnell & Olson (O'Donnell & Olson, 1981; Olson, 1982) provides a high-level graphics language and its associated interpretive software. It provides a general means of defining objects, drawable by line drawings, in such a way that these may be logically connected in groups or trees using a simple command language. Such a system may, for example, define a subunit protein of an icosahedral virus and define icosahedral symmetry, in such a way that modification of one subunit is expressed simultaneously in all subunits whilst preserving the symmetry, and simultaneously allowing the entire virus particle to be rotated. Such logical and functional relationships are established by the user through the medium of the *GRAMPS* language at run time, and a great diversity of such relationships may be created. The system is thus not limited to any particular type of structure, such as linear polymers, and has proved extremely effective as a means of providing animation for the production of cine film depicting viral and other structures. *GRAMPS* runs on all Silicon Graphics workstations under IRIX 4.0 or above.

3.3.3.1.5. *Takenaka & Sasada's system*

Takenaka & Sasada (1980) have described a system for the manipulation and display of molecular structures, including packing environments in the crystal, using a minicomputer loosely coupled to a mainframe. Their system is also capable of model building by the addition of groups of one or more atoms with a facility for monitoring interaction distances while doing so.

3.3.3.1.6. *MIDAS*

This system, due to Langridge and co-workers (Gallo *et al.*, 1983; Ferrin *et al.*, 1984) is primarily concerned with the display of existing structures rather than with the establishment of new ones, but it may modify such structures by bond rotations under manual control. It is of particular value in the study of molecular interactions since two or more molecules may be manipulated simultaneously and independently. Visual docking of molecules is greatly facilitated by the display of van der Waals surfaces, which may be computed in real time so that the turning of a bond in the underlying structure does not tear the surface (Bash *et al.*, 1983).

3.3.3.1.7. *Insight*

This system, originally due to Dayringer *et al.* (1986), has a functionality similar to *MIDAS*. It has been replaced by *Insight* II (current version 2.3.5). It appears to be well suited to the study of intermolecular relationships in docking and in structural comparisons, and it is able to make modifications to structures. Objects for display may be molecular or non-molecular, the former having an atomic substructure and the latter consisting of a vector list which may not be subdivided into referrable components. Map fitting with the current version has been reported.

3.3.3.1.8. *PLUTO*

PLUTO was developed by Motherwell (1978) at the Cambridge Crystallographic Data Centre (CCDC) for the display of molecular structures and crystal-packing diagrams, including an option for space-filling model style with shadowing. The emphasis was on a free format command and data structure, and the ability to produce ball-and-spoke drawings with line shadowing suitable for reproduction in journal publication. Many variant versions have been produced, with essentially the 1978 functionality, its popularity deriving from its ease of use and the provision of default options for establishing connectivity using standard bonding radii. It was distributed as part of the CCDC software associated with the Cambridge Structural Database, with an interface for reading entries from the database.

In 1993 Motherwell and others at the CCDC added an interactive menu and introduced colour and PostScript output. New features were introduced to allow interactive examination of intermolecular contacts, particularly hydrogen-bonded networks, and sections through packing diagrams (Cambridge Structural Database, 1994).

3.3.3.1.9. *MDKINO*

This system, due to Swanson *et al.* (1989), provides for the extraction and visualization of selected regions from molecular-dynamics simulations. It permits stereo viewing, interactive geometric interrogation and both forwards and backwards display of motion.

3.3.3.2. *Molecular-modelling systems based on electron density*

Systems described in this section require real-time rotation of complicated transparent scenes and all used vector-graphics technology in their original implementations for that reason, though many are now available for raster machines. In every case the graphics are the means of communication between the user and software possessing high functionality, capable of building a representation of a molecule *ab initio* and to alter it, change its shape and position it optimally in relation to an electron-density map, with due attention being paid to stereochemical considerations, by one or more of several approaches.

3.3.3.2.1. *CHEMGRAF*

Katz & Levinthal (1972) have developed a powerful modelling and display system for macromolecules known as *CHEMGRAF*. This system permits the definition of many atom types which includes bonding specifications, so that, for example, four types of carbon atom are included in the basic list and others may be added.

references