Visualization of diffraction pattern synchronized with rotation of crystal structure using AVS

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A crystal structure viewer (*CSV*) which visualizes 3D diffraction patterns synchronized with the rotation of a 3D crystal structure is developed by improving crystal lattice viewer (*CLV*) modules in the library of graphics software *AVS*. Five basic modules of *CLV*: generate colormap, transform tool, read dualxray and geometry viewer, are used in order to build the network modules of *AVS*. One of the modules, read dualxray, is modified for the building of *CSV*. The function of each module and scheme of the synchronization of rotation of a 3D crystal structure with its diffraction pattern are presented. A typical example of *CSV* application is shown using the simple molecule of $(SSCOC_2H_5)_2$ crystal.

Three-dimensional(3D) computer graphics software to help in the understanding of crystallographic procedure and to design crystal structure has been developed.[1,2] On the other hand, crystal lattice viewer (*CLV*) which visualizes the crystal lattice and corresponding reciprocal lattice using the graphics software Application of Visualization System (*AVS*)[3] was developed for the study of elemental X-ray crystallography.[4] One of the characteristic functions of *CLV* is to synchronize the crystal lattice with the reciprocal one. In this paper crystal structure viewer (*CSV*) which is an improvement of *CLV* is presented in order to visualize the synchronizing diffraction pattern with the rotation of a 3D crystal structure. The aim of *CSV* is to facilitate the understanding of elemental crystallographic knowledge, such as crystal point symmetry and space group extinction of diffraction intensity. Furthermore, as a structural analysis tool, *CSV* is expected to be useful for the modeling of complicated crystal structures that are difficult to determine, such as disordered structures, incommensurate structures and quasicrystals. In this paper the scheme of *CSV* and an example which illustrate the application of *CSV* to a simple molecule are presented.

AVS was developed as visualization software for data analysis and it has since been supported by Advanced Visualization System Inc. More than 230 *AVS* modules are used in scientific and technical fields, which represent independent computing elements performing specific functions. By combining the modules, users can create their own visualization system without writing programs. *AVS* is available for not only all major *UNIX* workstations and windows but also supercomputers. It requires at least 32 MB mainmemory and approximately 64 MB harddisk. In this work, the SUN SPARC 4/20 model 61 with Japanese Solaris 1.1.2 (SUN OS 4.1.4 JLE 1.1.4) was used, which includes 64 MB mainmemory, 2 GB harddisk and TGX+ graphics environment. It is connected to the file server S-4/690 with 128 MB mainmemory and 41.6 GB harddisk through the NFS (Network File System) of the Computation Center of our Institute: RIKEN.

Crystallographic data for computer graphics, i.e., lattice constant, crystal system, space group, atomic coordinates etc. for the crystal structure, and reciprocal lattice constant, intensity data with the reflection index, wavelength etc. for the diffraction pattern are obtained from Crystallographic Computation Program System (*UNICS-III*).[5] The crystal data communication in *CSV* with *UNICS-III* is done by forwarding the data to the input ports of **crystal pattern** modules in *CSV*. The data communication diagram is shown in Fig. 1.

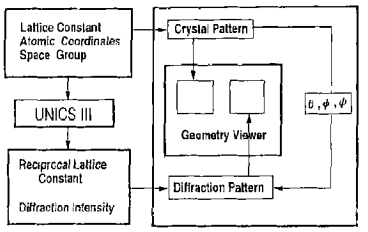

Fig. 1. System for data communication between *CSV* and *UNICS III*.

Consider the orthogonal Cartesian system (X, Y, Z) in the viewer windows. A basis of crystal lattice vectors (**a**,**b**,**c**) in the crystal viewer is set up referring to the Cartesian system. Reciprocal vectors (**a***,**b***,**c***) are referred to the Cartesian system through the crystal lattice basis (**a**,**b**,**c**). If a rotational operation around the X-,Y- or Z- axis (rotation angle of θ, ϕ or φ) is applied to the crystal pattern, the corresponding diffraction pattern begins to rotate simultaneously. Thus, the synchronization is designed such that the diffraction pattern follows the rotation of the crystal lattice. A network (Fig. 2) which has the functions mentioned above consists of four different modules, standard *AVS*-supported modules (**generate colormap** and **geometry viewer**), and those developed by Robinson and Hollander[3] (**read dualxray** and **transform tool**). **read dualxray** reads crystal and reciprocal lattice constants and generates their lattice patterns. **transform tool** in *CLV* plays an important role of synchronizing the window of the reciprocal lattice with that of the crystal lattice.

In order to improve *CLV* to *CSV*, it is only necessary to modify **read dualxray** for displaying the diffraction pattern of the crystal structure. Since the diffraction intensity data $I(hkl)$ and the reciprocal lattice constants are generated automatically from the crystal structure data, the diffraction pattern is easily generated by modifying **read dualxray**. Two

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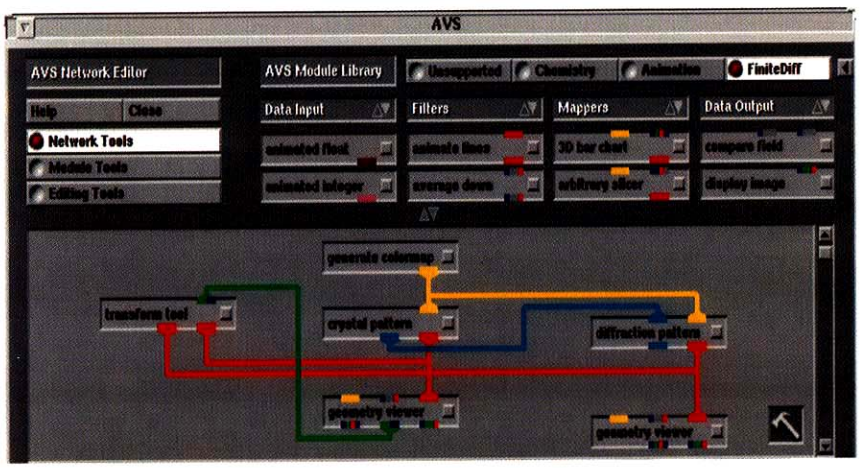

Fig. 2. Network modules in *CSV*.

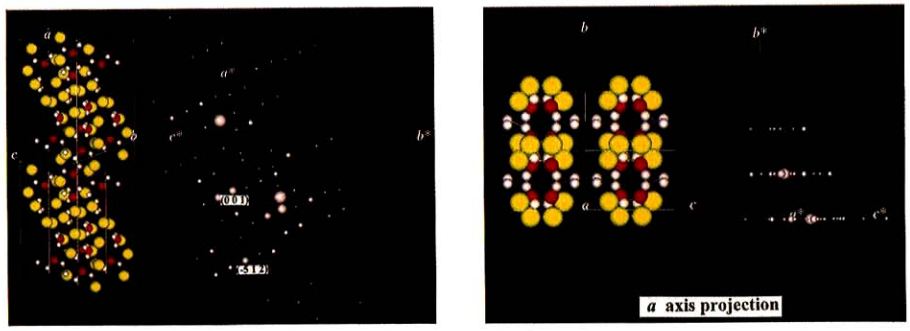

Fig. 3. Simultaneous visualization of diffraction pattern synchronized with rotation of crystal structure.

modified modules are **crystal pattern** for the crystal structure and **diffraction pattern** for the diffraction intensity pattern. These two pattern modules are visualized by **geometry viewer** of the supported module library of *AVS*. *CSV* is designed to visualize simultaneously the crystal and reciprocal lattice using the current transformation matrix of the Cartesian system in **geometry viewer**.

Thus *CSV* has a distinguishing characteristic that visualizes the diffraction pattern synchronized with the rotation of the crystal lattice as shown in Fig. 3. Left- and right-hand windows display crystal structure and diffraction pattern respectively. The following functions are added to the left- and right-windows viewer modules. First, the crystal structures are clearly displayed in the left windows by the following designs. Eight unit cell molecules are demonstrated for the crystal structure visualization. Each atom is represented by a sphere which is generated at the atomic coordinate center. The atom species are distinguished from each other by giving a size and color to each atom. A virtual atom with small size like a dot is put at each lattice point of the unit cell. The atom size can be chosen in proportion to the atomic radius. Atom labels and atom-atom bonds are presented so that the molecules in the unit cell can be conveniently visualized. Secondly, some idea of representation of diffraction pattern is given as follows: The intensity level represented by the radius of each sphere ranges from 5 to 100 steps. Some difficulty arises in the visualization of the diffraction pattern. Since too many 3D diffraction spots projected from one direction are shown all together on the display, the information of depth of the pattern seems to be lost. This is the reason why although the 3D space is a stereoscopic one, the dot pattern seems to be a projected one. In order to solve this problem, we set up a function called a *position-located* system which provides the input of reciprocal lattice indexes ($h\ k\ l$). By this means the corresponding index position in the reciprocal lattice is rapidly displayed using a new color completely different from those of other spots.

The test crystal data of simple molecule are chosen. Structure data is as follows:
Diethyldixanthogen, $(SSCOC_2H_5)_2$, lattice constant: a = 18.958, b = 4.394, c = 6.990 Å, β = 107.27°, *Space Group*: $P2/a$, number of intensity data: 353, number of atoms: 22.

The basic design of *CSV* is accomplished by modifying the modules in *CLV*. The final aim of *CSV* is to fit the crystal structure on the crystal pattern viewer to the experimental diffraction intensity $I_o(hkl)$. The geometrical operations in *CSV* are restricted to rotation around the virtual X-,Y- and Z-axes and magnification of the image at present; however, if *CSV* can incorporate a function of molecular micromanipulation or successive rotation of the bond angle and torsion angle of the local structure, *CSV* would facilitate real-time simulation of the crystal structure.

References

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