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MULTIPURPOSE CRYSTALLOGRAPHY SOFTWARE FOR MINERALOGISTS: *RECIPRO*

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X-ray, electron, and neutron diffraction crystallography have long been powerful analytical tools in numerous fields including mineral sciences. One of the challenges of these techniques is that novice crystallographers often have difficulty understanding the symmetry of a crystal structure from its diffraction pattern and the relationship between real space and reciprocal space. In particular, electron diffraction patterns are not intuitive because of the dynamical scattering effect, namely, multiple electron scattering, and atomic resolution S/TEM images are further modulated by the aberration of electromagnetic lenses. Thus, a detailed comparison between their precise simulations and experimental data is indispensable to achieve a quantitative analysis.

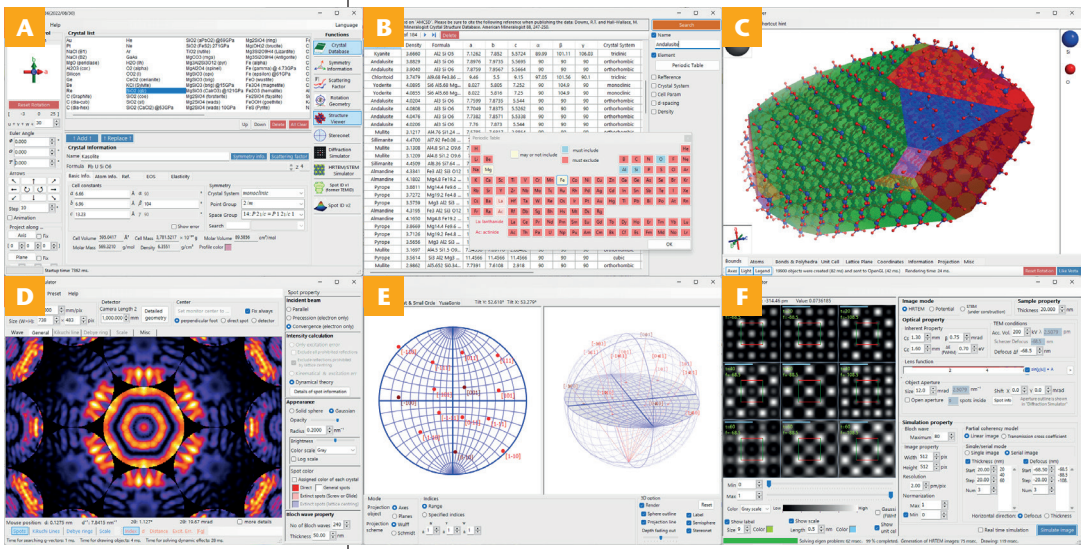
Given this background, we have developed *ReciPro*, a free and open-source GUI-based crystallographic software (Seto and Ohtsuka 2022) (Fig. 1A). It provides access to functions to explore crystal databases, visualize crystal structures and goniometer settings, simulate diffraction patterns and high-resolution microscope images (HRTEM and STEM), and analyze diffraction data. Although there exist other software with similar functions, none of them is as versatile and user-friendly as *ReciPro*. We have been developing this software continuously for about 20 years and made it open-sourced about three years ago. The software is already in use by hundreds of users in more than a dozen laboratories at universities and companies, contributing to the development of science and technology related to crystallography and mineralogy. Some of its features are briefly described below.

Crystal database: The built-in crystal database in *ReciPro* contains over 20,000 crystal structure models provided by the American Mineralogist Crystal Database (AMCSD) (Downs and Hall-Wallace 2003). The database is highly compressed (~9 MB) and included in the installation file; therefore, it is available in an offline environment (such as an isolated laboratory). Users can search for crystals in the database using various options (crystal name, contained elements, symmetry, and density) (Fig. 1B).

Structure viewer: *ReciPro* can visualise a crystal structure model as an attractive 3D graphic using an OpenGL architecture (Fig. 1C). Even complex crystal structures containing tens of thousands of atoms can be drawn smoothly in real time. By colouring the bounds plane, arbitrary crystal habits can also be represented. Furthermore, any lattice planes can be displayed, which will help beginners understand the concept of lattice planes in diffraction phenomena. The rotation, movement, and magnification/reduction of this 3D crystal structure can be freely controlled with mouse operations, and the rotation state is immediately reflected in the crystal orientation on other functional windows.

Diffraction simulator: *ReciPro* can simulate single-crystal diffraction patterns. Monochromatic X-rays, electrons, and neutrons are available as incoming waves (beams), and the kinetic energy can be freely configured. The energy of the characteristic X-rays from ^{1}H to ^{98}Cf is built-in. The crystal rotation (i.e., diffraction condition) can be controlled in this window and can be immediately synchronised with other windows. For X-ray and neutron sources, the simulations are based on the kinematical scattering approximation (i.e., single scattering approximation). The diffraction intensities are simply estimated from the square of the crystal structure factor amplitude and excitation error. For electron beams, dynamical scattering simulations of parallel-beam electron diffraction (selected-area electron diffraction (SAED) in experimental geometry), precession electron diffraction (PED), and convergent-beam electron diffraction (CBED) (Fig. 1D) based on the Bloch-wave method (Bethe 1928) are also supported. Algorithm optimization and CPU parallelization overcome the problem of computationally expensive dynamical simulations.

ReciPro is a completely free software distributed under the MIT license and runs on Microsoft Windows >7 or later with Microsoft .NET Desktop 6.0 runtime. *ReciPro* is installed by downloading and executing the setup file (ReciProSetup.msi) on the GitHub page https://github.com/seto77/ReciPro/releases/latest. All source codes and detailed documentation on usage have been published in the above GitHub repository. There are many other features that we have not covered here, such as stereonet projection (Fig. 1E) and HRTEM simulation (Fig. 1F), and we encourage our readers to try *ReciPro*.



Screenshots of *ReciPro*. (**A**) Main window. (**B**) Crystal database. (**C**) Structure viewer (SiO_2 quartz with {1000}, {10-11}, {01-11}, {11-21}, and {51-61} surfaces). (**D**) Diffraction simulator (CBED pattern of silicon [111] with 200-nm thickness). (**E**) Stereonet projection ($Mg_3Al_2Si_3O_{12}$ pyrope), (**F**) HRTEM simulator ($SrTiO_3$ tausonite [100]).

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