動力学的回折理論に基づく電子回折シミュレーションと鉱物への応用
Development of a software for electron diffraction simulation based on dynamical theory and its application to mineralogy

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Electron diffraction technique is widely used for the phase identification and crystal structure determination of Earth and planetary materials. Electrons are scattered by the positive potential inside the electron cloud, resulting that the interaction of electrons with matter is much stronger (10^6-10^7) than that of X-rays. This has the advantage that the diffracted electron beams have a high intensity and the patterns can directly be observed on the viewing screen of the electron microscope. The strong interaction, however, easily causes multiple scattering, and thereby the intensities of the reflections are much influenced by the dynamical effects. This makes structure determinations from electron diffraction more difficult and less reliable than that from XRD data. In order to treat the dynamical effects, a lot of computer resources of Fourier transform and/or eigenvalue problem are required, and consequently, such a dynamical analysis was limited to simple structured materials. However, that situation has been changing. In recent years, many-core CPUs can make a lot of computation possible. Moreover, with the rapid spread of field emission transmission electron microscopes (TEM) and sensitive detectors (CCD or CMOS), the quantitative analyses of electron intensities become available even from nanometer-sized minerals.

In the present study, the authors developed a GUI-based software, ReciPro, that simulates electron diffraction patterns using one of the dynamical theories, called the Bethe method (or Bloch wave eigenvalue method), in which the three dimensional eigenvalues of the electron wave function in a crystalline specimen are solved with the appropriate boundary conditions on the entrance and exit face of the crystal. By this method, the diffraction patterns (SAED and CBED) can be obtained with a good accuracy and speed regardless of the specimen thickness. Moreover, ReciPro provides following features: i) Loading any crystal structure including AMCSD (American Mineralogist Crystal Structure Database) database or COD (Crystallography Open Database). ii) Changing a specimen orientation and TEM conditions freely by a mouse operation. iii) Displaying Digital Micrograph file, the de facto standard of TEM image file format developed by Gatan inc., can be read and displayed. iv) Fitting diffraction spots by two dimensional pseudo-Voigt functions. v) Quantitative comparison of simulated and experimental diffraction patterns, and many more features. In the presentation, the authors will report examples of reproducibility of simulated diffraction patterns (SAED and CBED) for several minerals, and future prospects of this approach.

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