ElBis specifications

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FH electron optics

Overview

ElBis (electron beam and image simulator) is image simulation software for transmission electron microscopes (TEM and STEM) developed exclusively for Windows PCs equipped with a GPU (graphic processing unit). By using the parallel processing calculation of GPU, the TEM image and STEM image simulation calculation, which is generally considered to have a high load, is tens to hundreds of times faster than the calculation of a normal CPU (central processing unit) [1].

Another feature of ElBis is that it uses the extended TCC (transmission cross coefficient) [2] for aberration-corrected electron microscopes in the calculation of coherence in TEM images. With the expanded TCC, it is possible to correctly incorporate the effects of higher-order aberrations, which are essential for aberration-corrected electron microscope image calculations, into the calculations. This makes it possible to distinguish artifacts due to aberrations appearing in ultra-high resolution images from the sample structure.

Specifications

ElBis operating environment

, Windows (7 8 10), NVIDIA GPU (compute capability 3.0 or higher),
RAM 4GB (16GB or more recommended), monitor (14 inches or more),
Mouse with wheel function (used for parameter control)

Input parameters

Sample information

In the case of a single crystal sample

Unit cell size (lattice constant)
Crystal system designation (optional)

Space group designation (optional)
Types of constituent atoms and position coordinates
Debye factor (B factor)
Site occupancy
Sample thickness
Crystal orientation

In the case of supercell / special structure, amorphous structure, cluster, etc.

Supercell size (however, α = β = γ = 90.0 °, space group is specified as p1)
Types of constituent atoms and position coordinates
Debye factor (B factor)
Site occupancy
Sample thickness is the z-direction size of the supercell
The calculation direction can be specified arbitrarily on the GUI (graphic interface).

Microscope information

Acceleration voltage
Spherical aberration coefficient
Chromatic aberration coefficient
Out-of-focus amount (minus sign in the shortage direction)
Residual aberration after aberration correction (n-fold astigmatism (2,3,4,5,6), coma (2nd and 4th order), star, 3-lobe)
Angular source size
Energy spread of the source
Objective aperture size
Illumination aperture size
Brightness of the source
STEM detector placement (inner diameter, outer shape, position)

TEM image calculation

Both types of TEM image calculation can be calculated, single crystal and

supercell. In the case of a single crystal, the slice thickness is the equivalent point interval in the Z direction, and in the case of a supercell, any slice thickness can be specified. The internal procedure of the calculation is as follows. All of the following items are executed by GPU parallel computing.

Atomic scattering factor
Structure factor
Projected potential (volume of unit cell)
Dynamical electron diffraction (FFT multi-slice calculation)
Imaging calculation using TCC or envelope function (higher-order aberrations can also be considered in envelope calculation)

STEM (including CBD) image calculation

STEM image calculations apply only to supercells. HAADF (High Angle Dark Field) Image Meter
You can choose from two calculation methods: imaginary potential and frozen phonon.
The internal procedure of the calculation is as follows. All of the following items are executed by GPU parallel computing.

Absorptive form factor
Structural factor
Projection potential
Imaginary potential

Repeating the following calculation in the beam scan area

Atomic position fluctuation arrangement assuming frozen phonon / frozen phonon when instructed
New incident point arrangement of the beam
Dynamic electron diffraction (when the scattering intensity recording by beam shape and imaginary potential / imaginary potential is specified in each slice layer)
Detection signal intensity recording (recording of elastic scattering components in each slice layer)

Output image format

BMP 8Bit grayscale

Tiff 8bit / 16bit grayscale

Raw 32 bit floating point data

Other functions

Ronchigram calculation

Calculation of contrast transfer function (Imaginary part generated by odd symmetry aberration can be displayed)

Imaging calculation considering the orientation deviation of the single crystal sample

Imaging calculation considering the effect of axial misalignment of the optical system

Imaging calculation considering the effect of displacement of the objective diaphragm

Imaging calculation incorporating the effect of the phase plate

Imaging calculation considering the total amount of electron dose

Continuous image calculation by automatically changing the orientation of the cluster (supercell)

Sequential calculation using latitude and longitude maps

Calculation by random direction using random numbers

Calculation of amorphous embedding state (designation of density, B factor, atom type, etc.)

4D STEM function (CBD series storage corresponding to beam position, STEM image configuration with user defined arbitrary detector)

4D TEM function (calculation of hollow cone illuminated TEM image, storage of TEM image series corresponding to inclined beam)

CIF file (crystal data) and xyz file (Cluster data) can be read as specimen data

Composition

1 set of software and related files

1 set of licensed USB dongle

References

[1] F. Hosokawa, T. Shinkawa, Y. Arai and T. Sannomiya, Benchmark test of accelerated multi-slice simulation by GPGPU, Ultramicroscopy 158, 56-64 (2015).

[2] F. Hosokawa, H. Sawada, T. Shinkawa, T. Sannomiya, Image transfer with partial coherence for aberration corrected transmission electron microscopes, Ultramicroscopy 167, 11-20 (2016).

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