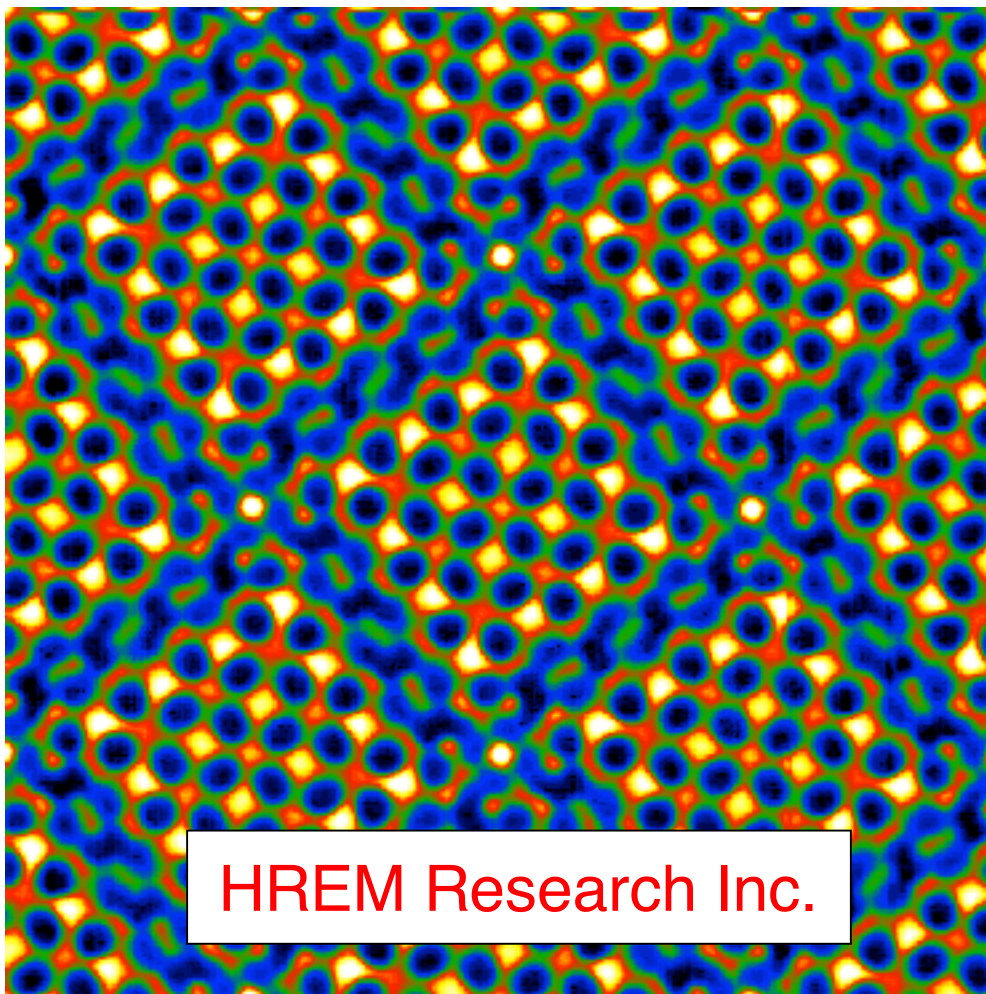
xHREM™

(*WinHREM*™/*MacHREM*™)

High Resolution Electron Microscope Image Simulation Programs



High Resolution Electron Microscope Image Simulation Programs

High Resolution Electron Microscopy (HREM) becomes an indispensable tool for understanding material properties or evaluating new materials at the level of atomic resolution. Due to increased demands for research and development of the new materials, an image simulation acquires more importance than ever before.

WinHREM™ /*MacHREM*™ is a suite of the high-resolution electron microscope image simulation programs that will work on a PC running on Windows or Mac OSX.

User Friendly Graphical Interface

WinHREM™ /*MacHREM*™ employs user friendly Data Generation Utilities based on the Graphical User Interface for Windows or Mac OS.

WinHREM™ /*MacHREM*™ is general-purpose software that can be used to simulate all the images expected from any crystal systems, defect structures and interfaces. Although data generation for such general-purpose software normally becomes complex, a novice user can easily generate his/her data by using the graphical Data Generation Utilities with minimum requirements for the special knowledge.

Reliable and Efficient Algorithm

Since electron microscope images critically depend on an electron-specimen interaction as well as aberrations of image forming lenses, the treatment of scattering based on dynamical theory and the treatment of aberration based on wave-optical theory are mandatory.

WinHREM™ /*MacHREM*™ emerges from the HREM image simulation programs based on FFT multislice technique developed at Arizona State University, USA (see References). This is one of the most reliable and efficient HREM image simulation programs.

Features of *WinHREM*™ /*MacHREM*™

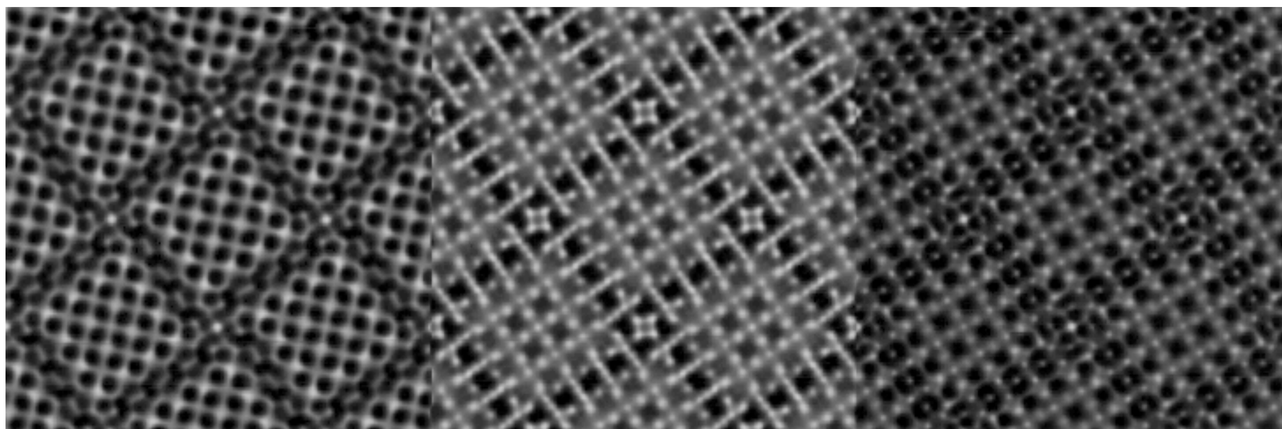
- Efficient algorithm based on Fast Fourier Transform (FFT)
- Applicable to any crystal systems, symmetries for an arbitrary beam direction
- Applicable to defects, interfaces and artificial supper-lattices
- Treatment of partial coherency based on the transmission cross-coefficient
- Efficient treatment of TDS using absorption potentials

References

K. Ishizuka and N. Uyeda, A New Theoretical and Practical Approach to the Multislice Method, Acta Cryst. A33 (1977) 740-749; K. Ishizuka, Contrast Transfer of Crystal Images in TEM, Ultramicroscopy 5 (1980) 55-65;
K. Ishizuka, Multislice Formula for Inclined Illumination, Acta Cryst. A38 (1982) 773-779; K. Ishizuka, A practical approach for STEM image simulation based on the FFT multislice method, Ultramicroscopy 90 (2001) 71-83.

High Quality Image Output

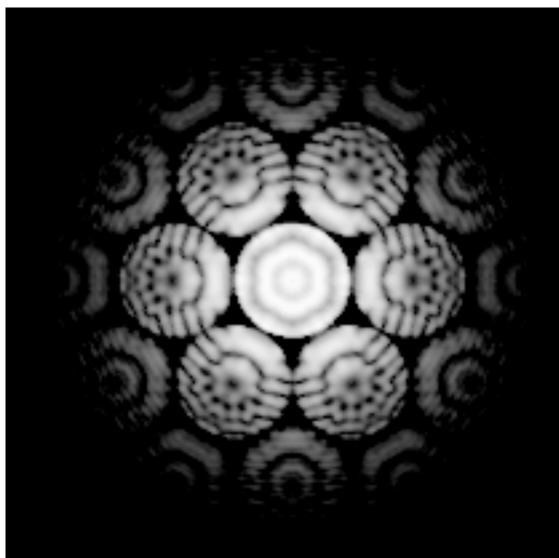
Numerical data such as projected potential, wave function propagating the specimen, simulated image intensities could be converted into a standard image format (Bit map, TIFF, etc.) and printed as high quality pictures by using Output Graphic Utilities. Photographic quality images as shown below could be obtained by using a high-quality printer.



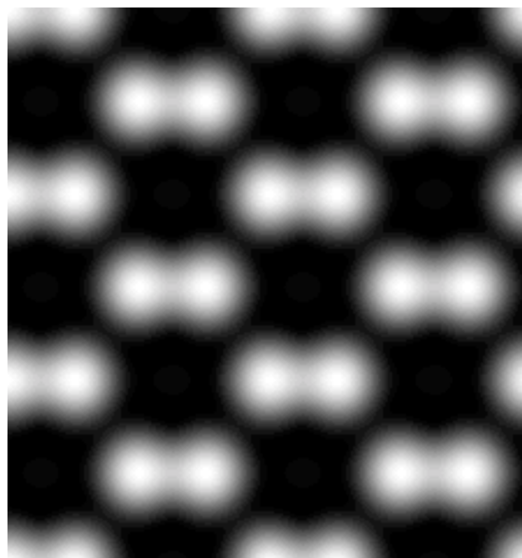
Simulated HREM images for tungsten niobate at 200 kV with Cs = 0.5 mm
Assumed thickness is 3.8nm; Defocuses from left to right are 42nm, 65nm and 83nm (under-focus)

Powered by Optional Functions

WinHREM™ /*MacHREM*™ could be extended its capabilities to simulate convergent-beam electron diffraction (CBED) patterns, diffuse scattering intensity distributions as well as scanning transmission electron microscope (STEM) images including high-resolution high-angle annular dark-field (HAADF) images by adding corresponding optional functions.



Simulated CBED pattern for Si [111]



Simulated HAADF image for GaAs [011]

WinHREM™ /*MacHREM*™ Specifications

1. Input data generation	Graphical User Interface (GUI) for Windows or Mac OS Standard values (Defaults) are preset for you
2. Scattering calculation	Efficient algorithm based on Fast Fourier Transform (FFT) Applicable to any crystal systems and symmetries Applicable to an arbitrary beam direction Applicable to defects, interfaces and artificial supper-lattices Possible to include the 3D effect (Upper layer-line effect) Possible to include the surface inclination effect Some important numbers Sampling points up to 256M (16kx16k)(1) Reflection index up to ±16k Atom species up to 20 from H to Cf Input atoms up to 1,000,000 Symmetry element up to 300 Phase grating up to 1000
3. Image calculation	Partial coherency: Envelope functions Transmission cross coefficients Exports numerical data for high-quality image graphics
4. Graphic utilities	Generation, archive and printing of gray-scale HREM images(2) Thickness plot or 2D gray-scale pattern of electron diffraction Phase contrast transfer function
5. Option functions	•Diffuse scattering intensity distribution •Convergent beam electron diffraction (CBED) pattern •Scanning transmission electron microscope (STEM) images

(1) Applicable sampling points depend on your computer memory (RAM) for the CPU intensive calculations. Efficient calculation can be performed by using a non-square sampling array (especially useful for an interface simulation).

(2) Bit map, TIFF and other format.

NOTE: These specifications may be altered to improve the performance without notices.

Please Contact to:

Send your inquiries about the price for a new license or an upgrade to:

support@hremresearch.com

HREM Research Inc.

14-48 Matsukazedai
Higashimatsuyama 355-0055, JAPAN
TEL/FAX (81) 493-35-3919
web site: www.hremresearch.com
email: support@hremresearch.com