

# Software for the discovery of new crystal structures

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A new software called QED (Quantitative Electron Diffraction), which has been licensed by Max Planck Innovation, has now been released by HREM Research Inc., a Japan based company, which is developing products and services in the field of High-Resolution Electron Microscopy. QED allows transmission electron microscopes to acquire novel kinds of data, opening up new possibilities in electron crystallography.

Transmission electron microscopes create magnified images of samples and are, in contrast to the [light microscope](#), even able to resolve individual atoms. When transmitting a beam of electrons through a crystalline sample such as a complex mineral or a crystallized protein, the electrons are being diffracted in a specific way. Collecting such diffraction patterns of a sample from several different directions uniquely identifies a specific crystal structure.

The new QED software now can control almost any [transmission electron microscope](#) to automatically collect so called LARBED (Large-Angle Rocking-Beam Electron Diffraction) patterns. LARBED patterns are comprised of a series of diffraction patterns collected for a large range of directions of the [electron beam](#). Although collected for a single specimen orientation such LARBED patterns provide 3-dimensional information and thus enable researchers to better extract information about the structure of [crystalline materials](#) in various fields of applications such as materials science, geology and life sciences.

LARBED is a patented procedure, which has been developed by Christoph Koch at the [Max Planck Institute](#) for [Intelligent Systems](#) (formerly Max Planck Institute for Metals Research) in Stuttgart, Germany. The advantage of LARBED is that it overcomes difficulties caused by multiple scattering of electrons passing through a sample. This dynamical scattering makes it, amongst other things, difficult to analyze the intensities of the

diffracted beam when using other methods based on electron diffraction. This leads to the loss of valuable information.

The new software for automated acquisition of LARBED patterns works by controlling the tilt angle and position of a collimated electron beam. The QED software compensates the beam shift with the help of the illumination system of the microscope. Thus data about characteristics from nano-sized samples can be collected. LARBED data contain an enormous amount of information about examined specimen, including specimen thickness, the absolute values of structure factors, the crystal symmetry even of very thin (

Provided by Max-Planck-Gesellschaft

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