Phase Extrapolation For Improving HRTEM Resoltion Using Maximum Entropy Blind Deconvolution Method and Gerchberg-Saxton Algorithm

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Abstract

Gerchberg-Saxton algorithm is applied to extend the HRTEM resolution using HRTEM image(s) and diffraction pattern. This algorithm restores spatial resolution by operating real space and reciprocal space projections cyclically. In our methodology , a generalized maximum entropy method (Kullback-Leibler cross entropy) to deal with weak scattering case is used as a real space (P1) projection . The lens contrast transfer function can be determined from the HRTEM crystal image(s). After P1 projection, not only the phases within the input frequencies are improved, but also the phases of the next higher frequencies are extrapolated. Square root of diffraction intensity from a diffraction pattern is then substituted for reciprocal space (P2) projection to complete a cycle operation of Gerchberg-Saxton algorithm. Cases of application of Gerchberg-Saxton algorithm to solve the atomic structure for $NiSi_2$/Si interfaces, $\Sigma 11$ Al_2O_3 and $\Sigma 5$ TiO_2 grain boundaies will be shown.