Efficient Computational Methods to Treat Multiple Scattering in Electron Diffraction by Nanostructures[1] G.M. GAVAZA, City U. Hong Kong, Z.X. YU, City U. Hong Kong, and Zhongshan U., L. TSANG, UW-Seattle, C.H. CHAN, S.Y. TONG, City U. Hong Kong, M.A. VAN HOVE, LBNL, Berkeley, and UC-Davis — Our purpose is to extend the capabilities of surface structure determination methods, such as Low Energy Electron Diffraction, so they can be used for nanostructures. To treat non-periodic systems, a cluster approach is used. The main computational challenge consists in solving a Ax=b matrix-vector equation of large dimension. Since matrix inversion is both memory and compute-time demanding, we have developed and tested two fast iterative methods to solve the above equation: the Sparse-Matrix Canonical Grid (SMCG) method shifts the atoms to a regular space grid and makes use of FFT transformations while the Multi-Level Singular-Value Decomposition (MLSVD) performs fast rank determination and SV decomposition of A. For both these methods, the compute time scales as N x $\log_2$N per iteration, where N is the number of atoms. These two methods complement each other in terms of the types of nanostructures that they handle best.

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Date submitted: 27 Nov 2004 Electronic form version 1.4