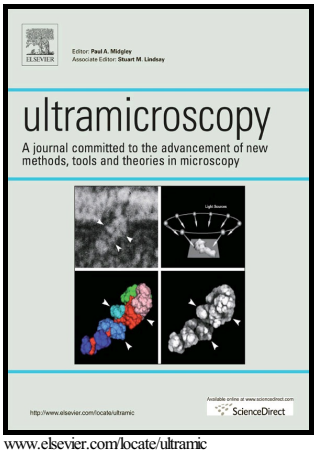
Significance of Matrix Diagonalization in Modelling Inelastic Electron Scattering

Z. Lee, R. Hambach, U. Kaiser, H. Rose



www.elsevier.com/locate/ultramic

PII: S0304-3991(16)30330-8
DOI: http://dx.doi.org/10.1016/j.ultramic.2016.11.011
Reference: ULTRAM12241

To appear in: *Ultramicroscopy*

Received date: 30 June 2016
Revised date: 13 November 2016
Accepted date: 17 November 2016

Cite this article as: Z. Lee, R. Hambach, U. Kaiser and H. Rose, Significance o Matrix Diagonalization in Modelling Inelastic Electron Scattering *Ultramicroscopy,* http://dx.doi.org/10.1016/j.ultramic.2016.11.011

Significance of Matrix Diagonalization in Modelling Inelastic Electron Scattering

Z. Lee[a], R. Hambach[a,b], U. Kaiser[a], H. Rose[a]

[a] *University of Ulm, Ulm 89081, Germany*
[b] *University of Jena, Jena 07743, Germany*

Abstract

Electron scattering is always applied as one of the routines to investigate nanostructures. Nowadays the development of hardware offers more and more prospect for this technique. For example imaging nanostructures with inelastic scattered electrons may allow to produce component-sensitive images with atomic resolution. Modelling inelastic electron scattering is therefore essential for interpreting these images. The main obstacle to study inelastic scattering problem is its complexity. During inelastic scattering, incident electrons entangle with objects, and the description of this process involves a multidimensional array. Since the simulation usually involves fourdimensional Fourier transforms, the computation is highly inefficient. In this work we have offered one solution to handle the multidimensional problem. By transforming a high dimensional array into twodimensional array, we are able to perform matrix diagonalization and approximate the original multidimensional array with its twodimensional eigenvectors. Our procedure reduces the complicated multidimensional problem to a twodimensional problem. In addition, it minimizes the number of twodimensional problems. This method is very useful for studying multiple inelastic scattering.

Keywords: inelastic scattering, MDFF, matrix diagonalization

1. Introduction

Electron scattering has been applied as a conventional method for determining and imaging nanostructures since several decades. Modelling electron scattering is essential for understanding the scattering process taking place during experiments, for example to interpret the contrast of high-resolution images obtained from modern transmission electron microscopes. The main obstacle for a quantitative analysis is the strong interaction between electron