

A new smoothing algorithm for statistical noise reduction

N. Moriya

Solid State Institute and Department of Physics, Technion – Israel Institute of Technology, Haifa 32 000, Israel

Received 15 May 1990 and in revised form 26 September 1990

A new, general, high quality smoothing algorithm is presented. It is based on a polynomial fitting of the real and imaginary components of the Fourier transformed spectra. Such fits, after inverse transformation into the real space, are shown to drastically reduce the statistical noise present in some experimental spectra and offer a fast and simple method for smoothing. The smoothing principles of this algorithm were applied, for demonstration of the quality of the fits which can be obtained, to Rutherford backscattering (RBS) and to particle induced X-ray emission (PIXE) spectra.

1. Introduction

Smoothing methods are needed for various applications, mainly for modeling and calculation procedures in many fields of applied physics where statistical noise is responsible for the spread of data points, as for example in Rutherford backscattering spectroscopy (RBS), particle induced X-ray emission (PIXE) or photoluminescence (PL) spectroscopy.

The importance of finding good smoothing algorithms is emphasized by the large number of different methods developed for this purpose. Such methods are, in most cases, based on averaging processes (as for instance the 5-point Savitsky–Goulay [1] smoothing operation), functional fitting [2,3] or filtering in the Fourier space of the analyzed spectrum [4,5]. Unfortunately, each of these methods suffers from basic disadvantages; it is almost impossible to obtain a reliable smoothed spectrum after gentle averaging iterations, while functional fitting is not always easy to apply on large arrays or on rapidly changing spectra. In the most common method, i.e. filtering analysis, it is a complicated matter to control the compensation in the loss of the high frequency elements caused by the filtering process, which is the reason for the imbalance in the height of the reconstructed spectra.

It is necessary therefore to find a method suitable for smoothing experimental spectra which includes statistical disturbances on one hand and keeps the physical information as free from distortions as possible on the other hand.

It is the aim of the present paper to present a new smoothing method and to show its potential for general spectra smoothing. The algorithm has been implemented in a form of a computer code which can be

adapted to any personal computer. Typical execution times (for a spectrum 1000 channels long) are few seconds when operated on an XT/PC microcomputer. Some examples are given and a detailed discussion on the advantages and limitations of this method is presented.

2. Principle

In the following, we present a method based on an analytical treatment of the frequency elements dispersed in the Fourier space. The basic idea behind this treatment is the use of a low degree polynomial fit to the real and imaginary parts of the Fourier transformed spectra in the frequency plane. These are shown to drastically reduce the statistical noise of the transformed spectra without introducing any serious distortion to the original data.

2.1. Theory

The application of Fourier analysis on a real function g_k at N discrete points x_k ($x = 0, \dots, N - 1$) is based on the following transformation [6,8]:

$$G_u = \sum_{k=0}^{N-1} g_k \exp(-i2\pi uk/N), \quad (1)$$

where k and u refer to the real and frequency spaces, respectively.

The function G_u which defines a one-dimensional space (so-called frequency space), represents the structure characterization of g_k in the regular space.

It is easy to show that the sum f_k of the two