

Application of Optimize Algorithm in EDXRF Spectrum Unfolding

Liu Mingbo¹, Liao Xueliang¹, Wang Guohua²

(1. NCS Testing Technology Co., LTD, Beijing, PR. China, 100081; 2. The Affiliated High School of Peking University, Beijing, PR. China 100080)

Abstract: On this work, we introduce an optimize algorithm to EDXRF spectrum unfolding process. Pure peaks, achieved by applying the smooth and debackground operation to raw spectrum, can be considered as the sum of several Gaussian peaks, which can be formulated by Gaussian functions with 3 parameters each, height, width and position. By alternating the values of the 3N parameters within certain boundary conditions, the error between theory function and raw spectrum can be smaller and smaller. In mathematics, this alternating process can be finished by Optimize algorithm. When we develop the algorithm by 3N parameters Conjugate Gradient Method and coding the program, an EDXRF spectrum of Pr/Nd solution was studied. Sum of 11 Gaussian peaks is very well closed to the raw spectrum composed of 11 L-series peaks of Pr and Nd, and the error calculated changed from 37.645 to 1.6994.

Keywords: Optimize Algorithm, EDXRF, Spectrum Unfolding, Conjugate Gradient Method