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Physica B 208&209 (1995) 175–176

PHYSICA B

EDA: EXAFS data analysis software package

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Abstract

The present paper describes the EXAFS data analysis software package, called EDA, originally developed by the author for IBM PC compatible computers. It consists of a set of interactive programs which allow to carry out all steps of the EXAFS data analysis procedure. There are two main differences from known packages. First, a significantly improved algorithm is used for atomic-like background removal in the EXAFS extraction procedure. Second, a model independent derivation of the radial distribution function from EXAFS, based on a maximum-entropy-like algorithm, is available.

The EDA software package [1, 2] consists of a set of interactive programs (EDAEES, EDAFT, EDAFIT, EDARDF and EDAPLOT), which allow to carry out all steps of the EXAFS data analysis procedure. Here only two of them (EDAEES and EDARDF) will be described.

The first program, called EDAEES, serves to extract the EXAFS signal $\chi(k)k^n$ from an X-ray absorption coefficient $\mu_{exp}(E)$. It uses significantly improved algorithm for atomic-like background removal. At the beginning, the background contribution $\mu_b(E)$ is approximated by a Victoreen polynom and subtracted from the experimental spectrum $\mu_{exp}(E)$: $\mu(E) = \mu_{exp}(E) - \mu_b(E)$. Further, the atomic-like contribution $\mu_0(E)$ is found in a *three-step* procedure to have a precise removal of the EXAFS-signal zero-line. This point is very important since unaccuracies in $\mu_0(E)$ can lead after Fourier filtering procedure to a distortion of the first shell EXAFS signal and an additional noise in EXAFS from outer shells. Besides $\chi(k)$ signal is usually multiplied in the EXAFS analysis by a factor k^n ($n = 1, 2, 3$), therefore the requirements to the extraction of $\mu_0(E)$ become even higher, since the error introduced by $\mu_0(E)$ into EXAFS signal will be magnified several times. On practice, the three-step procedure is realized as follows. At the first step, $\mu_0(E)$ is approximated by a polynom $\mu_0^I(E)$ (Fig. 1) of a power m_1 (the choice $m_1 = 2$ or 3 is recommended), which is then subtracted. The new function $\mu^I(E) = \mu(E) - \mu_0^I(E)$ is converted into the k-space and multiplied by a factor k^n with n equal or greater than the value, which one plans to use later in the analysis. At the second step, zero-line function $\mu_0^{II}(k)$ of $\mu^I(k)$ is approximated by a polynom of a power m_2, which has the value between 0 and 9, and the function $\mu^{II}(k) = \mu^I(k) - \mu_0^{II}(k)$ is calculated. The reason of the second step is that after convertion to the k-space with simultaneous multiplication by the factor k^n, the function $\mu^I(k)$ can have strongly distorted behaviour especially at high k-values. Thus, the idea of the first two steps is to obtain a function $\mu^{II}(k)$ which is enough well but not obligatory perfectly oscillating around zero within all range of k. At the third step, *precise* zero-line $\mu^{III}(k)$ of $\mu^{II}(k)$ is obtained by a cubic-smoothing-spline technique. As a result, the sought funciton $\mu_0(E)$ (Fig. 1) is calculated as a sum of $\mu_0^I(E)$, $\mu_0^{II}(E)$ and $\mu_0^{III}(E)$, and the EXAFS-signal $\chi(E)$ is determined as $\chi(E) = (\mu_{exp} - \mu_b - \mu_0)/\bar{\mu}_0$ where $\bar{\mu}_0$ is equal to μ_0 or properly normalized reference function μ_0^{ref}. Further, the EXAFS signal $\chi(E)$ is converted into k-space and can be multiplied by a factor k^n. The influence of the zero-line removal on $\chi(k)$ is clearly seen on its Fourier transform (Fig. 2).

The EDARDF program allows to determine *model-independent* radial distribution function (RDF) using

0921-4526/95/$09.50
SSDI 0921-4526(94)00663-6

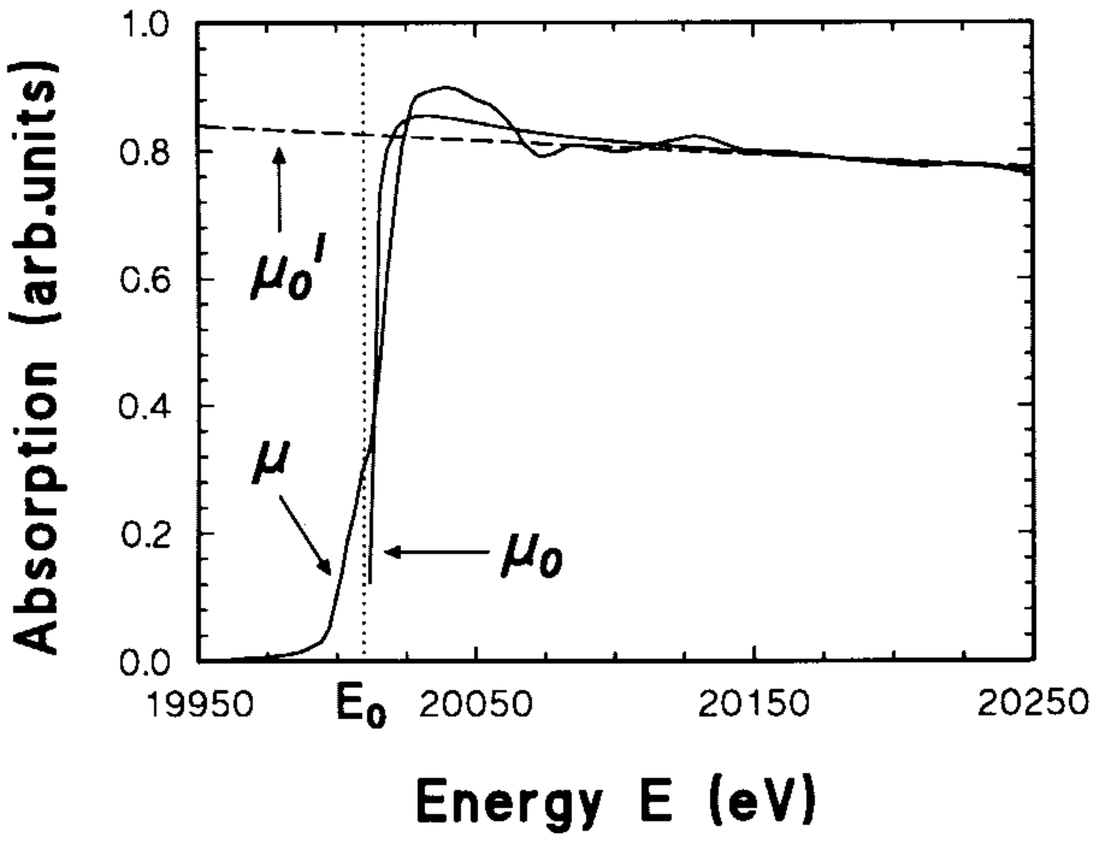

Fig. 1. Comparison between usual μ_0^I (dashed line) and μ_0 (solid line), obtained using approach described in present work, for the X-ray absorption spectrum μ of the Mo K-edge in MoO_3 [1].

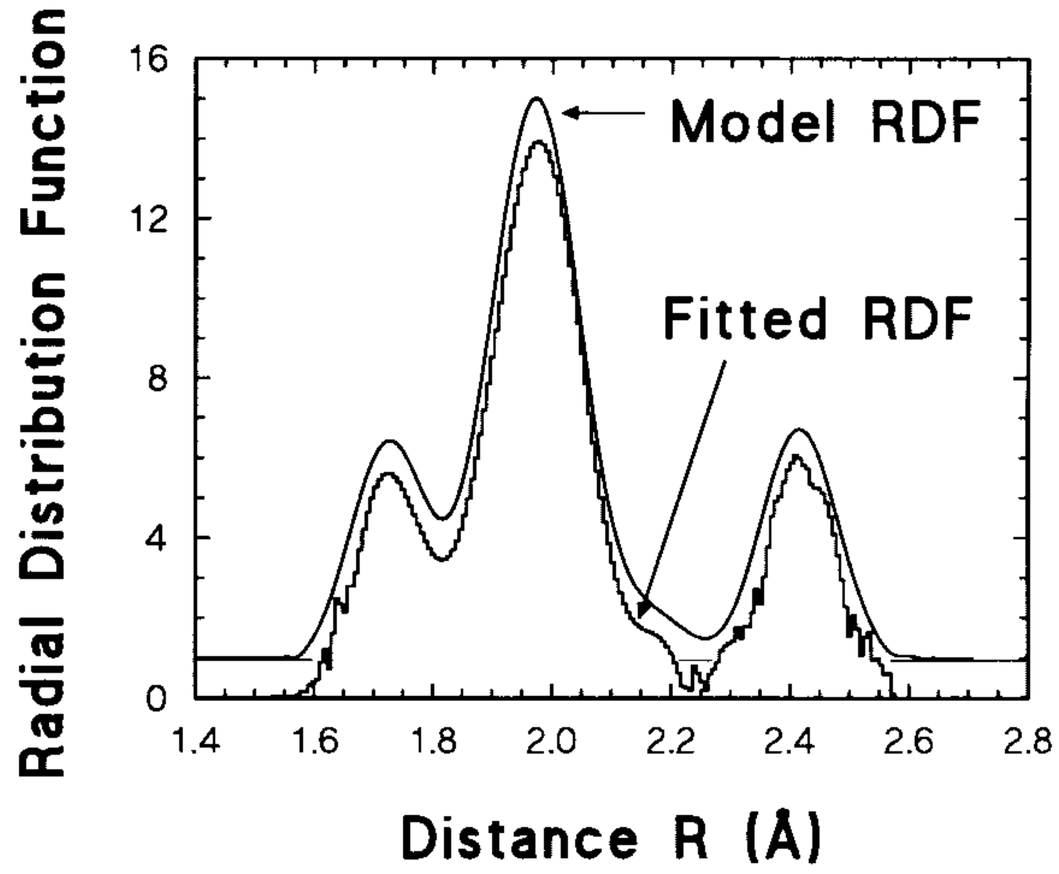

Fig. 3. Comparison between the true model RDF (smooth line) and the RDF found by the EDARDF code (histogram).

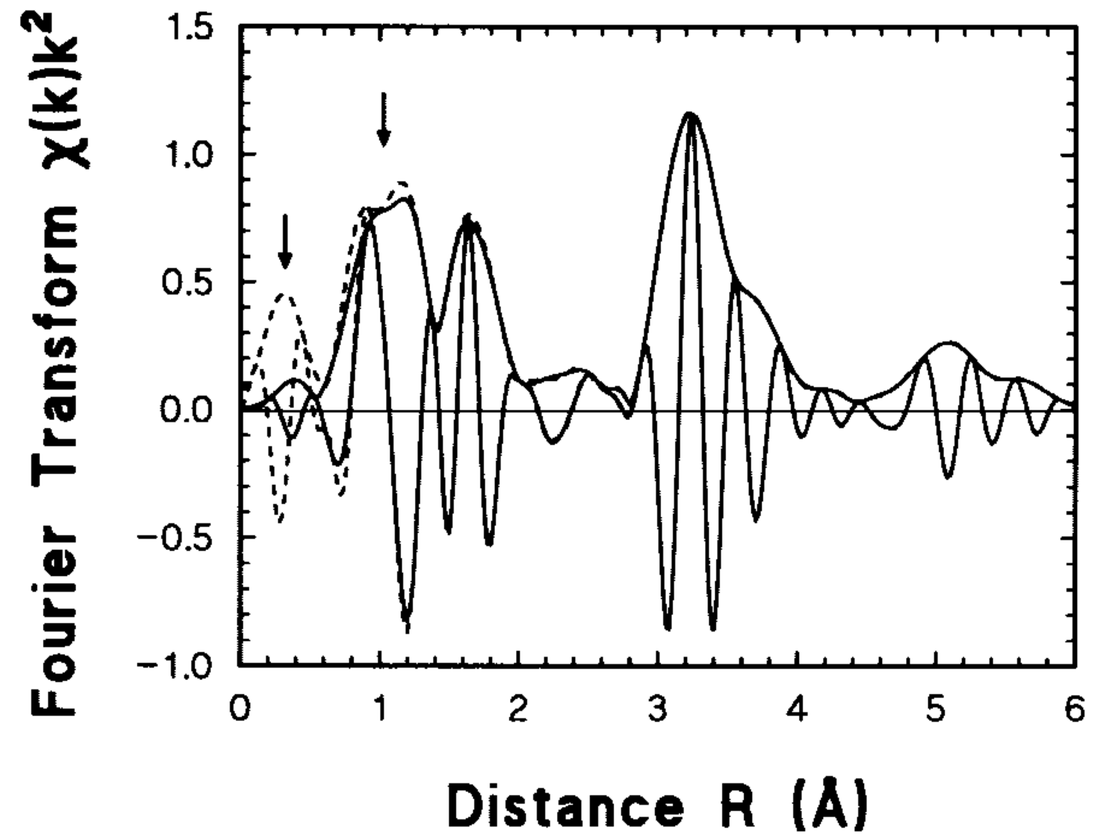

Fig. 2. Fourier transforms of the EXAFS signals extracted using the usual approach ($\mu_0 = \mu_0^I$) (dashed line) and the method described in present work ($\mu_0 = \mu_0^I + \mu_0^{II} + \mu_0^{III}$) (solid line).

theoretical or experimental backscattering amplitude and phase functions [3]. It is based on the maximum-entropy-like algorithm and is very suitable for the analysis of the first coordination shell EXAFS signal in highly locally disordered materials and systems with highly anharmonic behaviour, where the cumulant approach fails. For an arbitrary RDF $g(R)$, the general EXAFS expression in the curved-wave approximation is given by

$$\chi_{\text{model}}(k) = k^n S_0^2 \int_{R_{\min}}^{R_{\max}} \frac{g(R)}{kR^2} F(\pi, k, R) \times \sin(2kR + \phi(\pi, k, R))\,\mathrm{d}R$$

with usual meaning of all parameters. The starting approximation for $g(R)$ in the form of a histogram can have an arbitrary shape and is set on the grid from $R_{\min}$ to $R_{\max}$ with a step ΔR. To find true shape of RDF, the least-squares problem for the $\chi(k)$ function is solved: the amplitude of $g(R)$ is varying in each small interval ΔR till good agreement between experimental and model EXAFS signals will be reached (Fig. 3). The criterium of maximum–entropy allows to fix a smooth shape of the distribution.

References

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[3] J. Purans, A. Kuzmin, Ph. Parent and H. Dexpert, Physica B 208&209 (1995) 307, 373, 707.