

RAD, a program for analysis of X-ray diffraction data from amorphous materials for personal computers.

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1. System requirements

RAD runs under DOS 3.0x/later and WINDOWS 95/98/NT/ME/XP.
It requires 2 MB of core memory and a CGA/VGA/SVGA graphics card.

2. Getting started

Create a directory with a name of your choice. Copy **RAD.exe** as well as **scf1-98.dat** and **cyl** in it. The latter files contain the atomic scattering factors for x-rays and the absorption correction in case of cylindrical geometry.

RAD is the program itself (executable).

To start the program - type in RAD and press Enter.

Then select one of the options proposed - [S]etup, [R]eduction, [N]ormalization, [C]alculation, [D]os Utilities, [E]nd.

3. Running RAD

The radial distribution function analysis is usually carried out in several steps.
With the program RAD the steps are as follows:

Data [S]etup - creates a file containing physical quantities and parameters describing the sample and the particular diffraction experiment. Simply provide all parameters as requested. The file created is a text one and, if necessary, can be modified (outside **RAD**) using a text editor.

Data [R]eduction - corrects for absorption, polarization and background scattering. File(s) with raw experimental and background data as well as the already created parameters' file are needed as input data. The XRD data files are two column files - the first column is the Bragg angle (in 2 theta) or the scattering vector Q (in \AA^{-1}). The second - the corresponding intensities in counts per second. The corrected X-ray diffraction data are stored in a file (in text format) to be used in the next step.

Data [N]ormalization - the already corrected XRD data is brought (normalized) into absolute(electron) units. Then, the so-named reduced structure factor $Q[S(Q)-1]$ is calculated. A file with the corrected XRD data and the parameters' file are needed as input data. The reduced interference function data is stored in a data (text) file.

HINT: Apply the "high-angle" normalization method at first. Then refine the normalization constant by trial and error, if necessary.

RDF [C]alculation - The atomic distribution functions $G(r) = 4\pi r[\rho(r)-\rho_0]$, $g(r) = \rho(r)/\rho_0$ and $RDF = 4\pi r^2 \rho(r)$ are calculated by Fourier transforming the experimental reduced structure factor. Text files with $G(r)$, $g(r)$ and/or RDF data are created.

[D]OS utilities - allows DOS commands to be executed without leaving RAD.
To return to RAD - type Exit.

[E]nd of job - exits the program RAD (or CTRL-C at any time).

For more details about the theoretical background and computational algorithms involved see: **V.Petkov, J. Appl. Cryst. 22 (1989) 387-389.**

4. Test example

Files illustrating the radial distribution function analysis of XRD data from Gd₄Al₃ metallic glass are provided. For more information see: **PETKOV et al. J. Non-Cryst. Sol. 108 (1989) 75.**

Files:

GdAl.raw - raw X-ray diffraction data (in Bragg angles)

AIR.raw - air (background) scattering data (in Bragg angles)

GdAl.par - physical quantities and parameters describing the sample and the particular experimental conditions. Created by running Data [S]etup.

Parameters in GdAl.raw - $\rho_o = 0.0392$ [atoms/Å³], Filtered Mo K α radiation with $\lambda=0.709$ Å, $\mu t=0.6775$, reflection geometry, $c\%[Gd] = 0.57$, $c\%[Al]=0.43$.

GdAl.cor - corrected XRD data. Created applying Data [R]eduction.

GdAl.rif - reduced structure factor Q[S(Q)-1] for Gd₄Al₃. Calculated applying Data [N]ormalization.

GdAl.rdf - reduced radial distribution function G(r) for Gd₄Al₃ metallic glass calculated by running RDF [C]alculation. No damping applied.

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Any remarks and suggestions are welcome. Please, contact:

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