**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.
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 and copy **RAD.exe** and **scf1-98.dat** in it. The latter file contains the atomic scattering factors for x-rays, the former 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. That is all. The file created is a text one and so it can be redacted by any text editor, if necessary.

Data [R]eduction - correction for absorption, polarization and background scattering is carried out. File(s) with raw experimental and background XRD 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 $Å^{-1}$). 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 preliminary corrected XRD data and the parameters' file are needed as input data. The reduced interference function data is stored in a data 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 $G(r) = 4\pi r[\rho(r)-\rho_o]$, $g(r)= \rho(r)/\rho_o$ and $RDF = = 4\pi r^2\rho(r)$ are calculated by Fourier transforming the experimental reduced structure factor. 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).

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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 $Gd_4Al_3$ 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/ Å$^3$], Filtered Mo $K_\alpha$ 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 in the step Data [R]eduction.
GdAl.rif - reduced structure factor Q[S(Q)-1] for $Gd_4Al_3$. Calculated in the step Data [N]ormalization.
GdAl.rdf - reduced radial distribution function G(r) for $Gd_4Al_3$ metallic glass. Calculated in the step RDF [C]alculation. No damping applied.

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Any remarks and suggestions are welcome. Please, contact:

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