

DDM, Derivative Difference Minimization program version 1.5

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WWW:

http://www.icct.ru/eng/content/persons/Sol_LA/ddm.html

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http://www.geocities.com/l_solovyov/ddm.html

The DDM program for powder diffraction analysis implements the Derivative Difference Minimization method [1, 2] of full-profile fitting that has been developed recently as a background-independent alternative to the conventional Rietveld refinement scheme. The method is based on the minimization of the difference profile curvature and modulations that allows excluding the background line modeling from the refinement and thus reducing systematic errors caused by inadequate background definitions. The program includes both DDM and Rietveld refinement procedures for X-ray and neutron powder diffraction data, the Le Bail [3] and the DDM profile decomposition [4] routines, the quantitative phase analysis and the size-strain calculations.

In the new release of DDM the space group interpretation and reflection generation routines were changed to more flexible and reliable ones. Both Hermann-Mauguin and Hall notations with various nonstandard settings are recognized. The valid symmetry restrictions on all variable parameters are imposed automatically by the program.

The DDM algorithm includes three different weighting schemes designed for various expected levels of systematic errors in the experiment. For the Rietveld refinement the enhanced weighting scheme proposed by Toraya [5] is added.

The DDM suite is extended by a Fourier calculation utility DDMap.

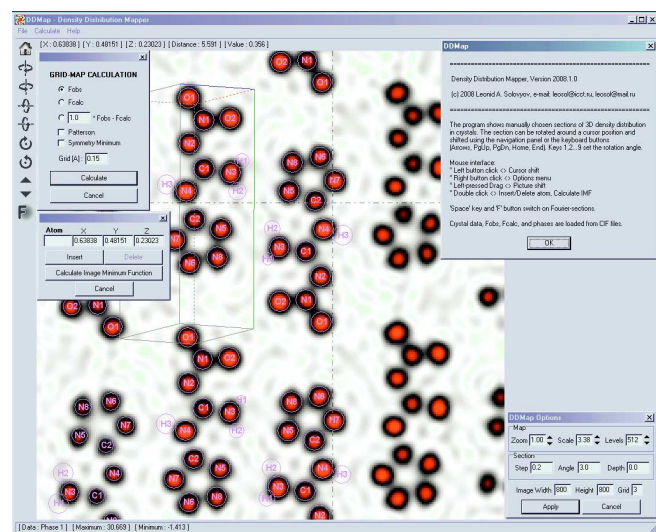


Figure 1. DDMap interface.

This program reads crystal data and structure factors with (optional) phases from a standard crystallographic information file (CIF), calculates Fourier and Patterson maps including the Symmetry and the Image minimum functions and allows viewing manually chosen sections of the 3D

distribution map. The CIF file is generated by DDM at the final stage of structure refinement and/or profile decomposition. DDMap recognizes all valid formats of CIF and can be used as a standalone Fourier calculator and viewer. It also generates GRD-files readable by 3D viewers such as MCE [6] and Vesta [7]. The structure model may be built and modified within DDMap by adding and removing atoms. The atomic coordinates are imported from CIF and saved in DDM format.

Additional new features:

- Automatic procedure for the initial scale factor (SF) estimation which is called by setting SF=0 for a selected phase.
- New asymmetry parameter P2 responsible for the lattice-gradient effect.
- CIF-output is directed to a single file ddm_cif.cif.
- Holes in the refinement codeword sequence are removed automatically.
- The site multiplicity is automatically calculated when it is set to -1.

The graphical user interface (GUI) for DDM is under construction and will be included in future releases. The program package includes a configuration for the freely available Programmer's File Editor (PFE) [8] that facilitates integrating DDM with graphical utilities such as WinPlotr [9], DDMap and structure viewers within the PFE shell. An example of the PFE-DDM interface demonstrating a combined use of DDM, WinPlotr and Mercury [10] viewers is illustrated by Figure 2.

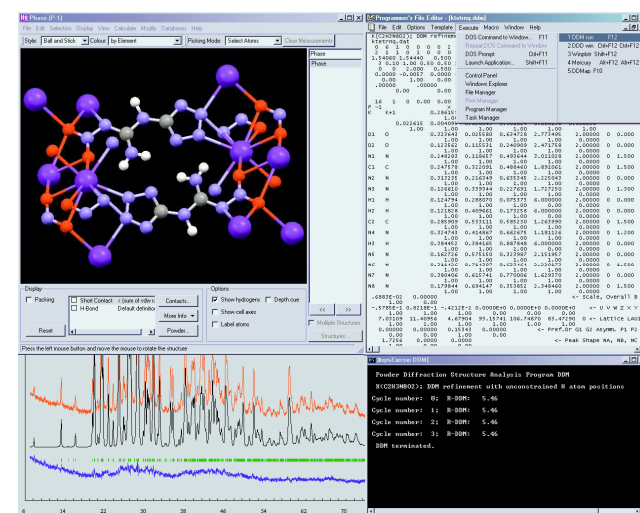


Figure 2. PFE-DDM shell combining WinPlotr and Mercury viewers.

The DDM executable, Fortran source code, documentation and examples are available at the above web addresses.

- [1] L. A. Solovyov, *J. Appl. Cryst.* 37 (2004) 743.
- [2] L. A. Solovyov, *Powder Diffraction Theory and Practice*, ed. R. E. Dinnebier and S. J. L. Billinge (2008) 282.
- [3] A. Le Bail *et al.*, *Mater. Res. Bull.* 23 (1988) 447.
- [4] L. A. Solovyov *et al.*, *Acta Cryst. B* 61 (2005) 435.
- [5] H. Toraya, *J. Appl. Cryst.* 31 (1998) 333.
- [6] www.vscht.cz/min/mce
- [7] www.geocities.jp/kmo_mma/crystal/en/vesta
- [8] www.lancs.ac.uk/people/steveb/cpaap/pfe
- [9] www-llb.cea.fr/fullweb/winplotr/winplotr.htm
- [10] www.ccdc.cam.ac.uk/products/mercury