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BilKristal 4.0: A tool for crystal parameters extraction and defect quantification

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ABSTRACT

In this paper, we present a revised version of *BilKristal 3.0* tool. Raycast screenshot functionality is added to provide improved visual analysis. We added atomic distance analysis functionality to assess crystalline defects. We improved visualization capabilities by adding high level cut function definitions. Discovered bugs are fixed and small performance optimizations are made.

New version program summary

Program title: BilKristal 4.0

Catalogue identifier: ADYU_v4_0

Program summary URL: http://cpc.cs.qub.ac.uk/summaries/ADYU_v4_0.html

Program obtainable from: CPC Program Library, Queen's University, Belfast, N. Ireland

Licensing provisions: Standard CPC licence, http://cpc.cs.qub.ac.uk/licence/licence.html

No. of lines in distributed program, including test data, etc.: 370130

No. of bytes in distributed program, including test data, etc.: 8350850

Distribution format: tar.gz

Programming language: C, C++, Microsoft .NET Framework 2.0 and OpenGL Libraries.

Computer: Personal Computers with Windows operating system.

Operating system: Windows XP or higher.

RAM: 20–60 Megabytes.

Classification: 8.

External routines: Microsoft .NET Framework 2.0. For the visualization tool, graphics card driver should also support OpenGL.

Catalogue identifier of previous version: ADYU_v3_0

Journal reference of previous version: Comput. Phys. Comm. 187 (2015) 266

Does the new version supersede the previous version?: Yes

Nature of problem: Determining the crystal structure parameters of a material is a very important issue in crystallography. Knowing the crystal structure parameters helps the understanding of the physical behavior of material. For complex structures, particularly for materials which also contain local symmetry as well as global symmetry, obtaining crystal parameters can be very hard.

Solution method: The tool extracts crystal parameters such as primitive vectors, basis vectors and identifies the space group from atomic coordinates of crystal structures.

Reasons for new version: Additional features, Performance optimizations, Minor bug corrections.

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Summary of revisions:

- Raycast screenshot functionality is added to the visualization tool. A raycasting algorithm similar to the one described in [4, 6] is used. The algorithm is multi-core parallelized as described in [5].
- Atomic distance analysis functionality is added. Tool can analyze the crystal structure and give statistical information of atom to atom distances.
- In the visualization tool, high level cut function support is added. Users can define cut functions, not just as cut-planes but with more complex functions as well.
- Automatic primitive vector and basis vector selection options are added. This way the system selects the simplest primitive and basis vector alternatives and continues without interrupting the user.
- In the visualization tool, an unused log file was being created and a redundant configuration file was being used. These issues are corrected.
- Dead-codes are removed to improve clarity.

Restrictions: Assumptions are explained in [1, 2, 3]. However, none of them can be considered as a restriction to the complexity of the problem.

Running time: The tool was able to process input files with more than a million atoms in less than 20 seconds on a PC with an Athlon quad-core CPU at 3.2 GHz using the default parameter values.

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