MedeA Pearson

Essential Tool for Scientists and Engineers Working With Inorganic Materials

MedeA®[1] *Pearson*, the world's largest experimental database for inorganic structures, delivers crystallographic data extracted from nearly 100,000 publications. *MedeA Pearson* provides detailed crystal structure information for alloys and intermetallics, ceramics, and minerals.

At-a-Glance

The integration of *MedeA Pearson* with all *MedeA modules* accelerates project execution by providing direct structure input for property predictions and high-throughput simulations.

Key Benefits

- Seamless integration with *MedeA InfoMaticA*, *MedeA* workflows, and *MedeA* compute engines
- Provides project planning with exhaustive account of chemical inventory
- The crystal structure data are processed and evaluated by expert scientists

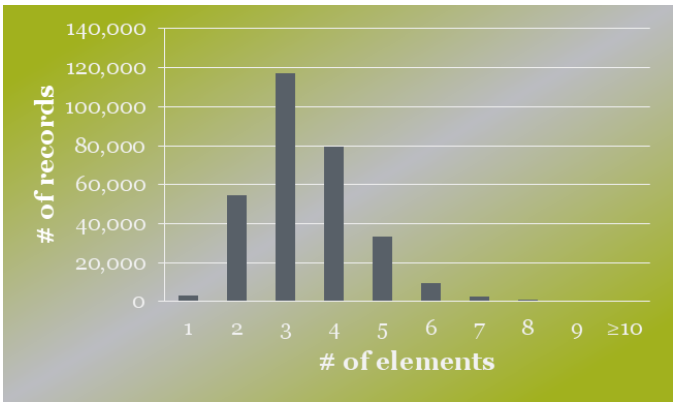

Figure 1: MedeA Pearson - *number of records by constituent count*

With a particular focus on alloys and intermetallics, *MedeA Pearson* provides exhaustive coverage of crystal structure data for inorganic compounds obtained from neutron diffraction and X-ray diffraction (XRD) powder diffraction measurements. Together with *MedeA InfoMaticA*, *MedeA Pearson* is an ideal starting point for building atomistic models of bulk phases, defect structures, surfaces, and interfaces.

'An exhaustive resource of experimental crystal structure data, in particular for alloys and intermetallics.'

Specifications

- World's largest critically-evaluated, 'non-organic database'
- Excellent coverage of alloys and intermetallics
- Encompasses more than 300,000 structure records of more than 95,000 different phases
- About 173,000 distinct chemical formulas
- 1 GB database file stored on disk

Key Features

- Provides on-disk, cross-database search in combination with *MedeA InfoMaticA*
- Quick, efficient structure retrieval using an intuitive, menu-based query language
- Regular database updates, along with *MedeA* updates

Properties

- Detailed information of lattice parameters, symmetry (space group), and bibliographic reference
- Meta data, such as cell parameters, as a function of pressure or concentration
- Atomic coordinates, interatomic distances and angles
- Atomic coordination
- Pair correlation function
- X-ray diffraction (XRD) powder pattern (radiation source dependent)

[1] MedeA and Materials Design are registered trademarks of Materials Design, Inc.

Required Modules

- *MedeA Environment* (includes *MedeA InfoMaticA*)

Recommended Modules

- *MedeA COD*
- *MedeA MSI Eureka*
- *MedeA ICSD*
- *MedeA NCD*
- *MedeA VASP GUI*
- *MedeA VASP*
- *MedeA HT-Launchpad*

Find Out More

Learn more about *MedeA InfoMaticA* in the video tutorial: How to Calculate Elastic Constants with MedeA VASP 5 on the Materials Design Youtube Channel.

For further information on the *MedeA Pearson* and on how *MedeA* can help you in your work, visit the Materials Design Youtube Channel, or contact us directly by email or phone.

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