

Adaptable Web-based Virtual X-ray Powder Diffraction Laboratory for Education and Professional Training

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The development of this virtual X-ray Powder Diffraction Laboratory (v-XRPD Lab) was inspired by the following motivations:

- Lack of hands-on experimentation associated with today's online engineering, technology and natural science courses which is an integral and mandatory part of any traditional science or engineering curricula.
- Limited availability of advanced research X-ray equipment for educational purposes due to its uniqueness, safety concerns, and, especially in developing countries, high price tag.
- Highly automated contemporary research and analytical equipment executes most tasks without user participation. This results in shallow understanding by many students and new users on the impact of experimental data collection factors on data accuracy, method limitations, and, hence, their inability to correctly estimate reliability of the results.
- In addition, actual experimentation often require more time than some programs can allocate to studying the corresponding subjects.

The described v-XRPD Lab helps overcome the above-mentioned problems, addresses the demands of distance and blended education, and meets learning habits of today's students. It enables users to perform authentic experiments online, using a multifunctional virtual XRPD diffractometer. The equipment realistically imitates the design and operation of a typical Bragg Brentano reflection mode geometry diffractometer and also includes educational analytical software. Experimental data can be collected and handled manually or automatically. This allows students to practice concepts, tasks, and equipment operation in a manner that cannot be achieved using actual totally automated equipment. Virtual data can be exported to popular analysis software as well. To enhance the v-XRPD-lab experience, it is being linked with a limited number of ICDD PDF[®] cards.

The v-XRPD Lab includes an open collection of samples available for carrying out virtual experiments. The diffractometer can work with CIF files obtained from the ICDD, ICSD, and CCDC databases. XY formats produced by many vendor's software, and some plain text files as well. The open collection of virtual samples available for online experimentation includes alloys, ceramics, polymers, nanostructured materials, thin films and even human kidney stones.

A complimentary authoring tool enables instructors to create their own experiments and add new samples to the collection.

The v-XRPD Lab has been used in several U.S. and international universities for teaching materials science and engineering courses as follows: (i) as the only tool for lab practice on the relevant subjects by the students who have no access to real equipment including Massive Open Online Courses (MOOC) students; (ii) for hybrid experimentation in combination with equipment; (iii) for preparing students and tech personnel to effective and meaningful hands-on practice in actual X-ray labs; (iv) for performance-based assessment of students' and trainees understanding and their ability to apply acquired knowledge and skills for performing experiments and solving practical tasks; (v) and for lecture demonstrations.

