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The Use of Web-based Virtual X-Ray Diffraction Laboratory for Teaching Materials Science and Engineering

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ABSTRACT

A virtual X-Ray Laboratory for Materials Science and Engineering has been developed and used as a flexible and powerful tool to help undergraduate and graduate students become familiar with the design and operation of the X-ray equipment in visual and interactive ways in order to learn fundamental principles underlying X-ray analytical methods. The virtual equipment and lab assignments have been used for: (i) authentic online experimentation, (ii) homework and control assignments with traditional and blended courses, (iii) preparing students for hands-on work in physical X-ray labs, (iv) lecture demonstrations, and (v) performance-based assessment of students' ability to apply gained theoretical knowledge for operating actual equipment and solving practical problems. Students have also used the virtual diffractometer linked and synchronized with an actual powder diffractometer for blended experimentation. Using the associated learning and content management system (LCMS) and authoring tools, instructors kept track of students' performance and designed new virtual experiments and more personalized learning assignments for students. The lab has also been integrated with the MITx course available on the massive open online course edX platform for Massachusetts Institute of Technology for undergraduate students.

INTRODUCTION

Today's advanced research equipment is typically fully computerized with most tasks executed routinely without user participation. Procedures such as equipment calibration, data collection, data handling and interpretation are performed automatically. While this provides enormous benefits for researchers, it also creates a number of substantial educational drawbacks and limitations. Except sample preparation and installation, all procedures related to pattern analysis, measurements, peak indexing, etc. are executed by a computer without student involvement. This is one of the reasons why many students experience difficulties in assessing applicability and limitations of methods, and factors affecting data accuracy. Hence, they cannot correctly estimate the reliability of the results. In addition, many students, especially those enrolled in on-line or large-class science and engineering courses, lack opportunities for hands-on practice and experimentation that involve X-ray equipment due to limited availability and accessibility of this expensive equipment for educational purposes.

Although there are plenty of free and commercially available powerful research software packages for X-ray diffraction and crystal structure modeling, there is a lack of comprehensive and interactive tools designed specifically for facilitating not only research or training on specific equipment, but first and foremost, the learning process.

To overcome some of these problems, address the demands of distance and blended education, and match the learning habits of today's students, the customizable virtual X-Ray Laboratory (v-XRLab) for materials science and Engineering education has been developed [1]. This powerful and flexible educational tool aims to help students gain knowledge and practical skills that are difficult to get using a real computerized X-ray equipment. The v-XRLab enables undergraduate and graduate students to perform authentic experiments online, using fully functional virtual replicas of actual X-ray equipment. Along with associated cyber infrastructure and interactive multimedia resources, it provides students with an opportunity to practice concepts, tasks, and equipment operation anytime and anywhere.

This dramatically differentiates v-XRLab from other XRD simulations [2, 3] that focus on specific models of commercial diffractometers and do not allow users to interactively explore equipment parts and systems or choose samples from a rich library/collection, not to mention creating and scanning their own real or calculated samples.

DESCRIPTION OF VIRTUAL X-RAY LABORATORY

The v-XRLab enables learners to become familiar with nondestructive research and testing methods widely used in science and industry, to explore the design and operation of X-Ray equipment and its major parts, and to learn underlying scientific and engineering principles and laws. Through on-line and blended activities, students gain practical skills required for conducting actual experiments, mastering to collect, analyze and interpret experimental data, and examining the instrumental factors affecting data accuracy.

The v-XRLab includes simulations, an open library of samples, and expandable sets of online experiments. It also contains supplementary educational resources, authoring tools, learning and content management system (LCMS), and cyberinfrastructure. Highly interactive simulations authentically reproduce equipment design and operation and realistically model relevant physical processes. v-XRLab includes educational analytical and modeling software as well.

An online experiment is a self- directed learning activity that is composed of one or more core simulations and includes a scenario/assignment, worksheets, assessments, and, most importantly, detailed guidelines for students. The student is expected to follow a thorough set of step-by-step instructions to accomplish an educational assignment. Virtual activities may also incorporate various multimedia resources such as prerecorded video lectures, animations, quizzes, links to databases, among others. These resources can be called up within virtual experiments to provide needed information and facilitate "just-in-time" learning opportunities. Each experiment focuses on a particular task and aims to achieve specific learning objectives.

ONLINE EXPERIMENTS

Over the course of an online experiment, students have the opportunity to- complete all of the procedures required - in the similar experiment performed using an actual X-ray equipment. The experiments developed by the authors of this paper and their colleagues were substantially different due to the great diversity of course subjects, student majors, educational goals and settings. Below we will outline the common steps of most experiments using the virtual X-ray powder diffractometer (v-Diffractometer). Screenshots in Figure 1 illustrate the concept of the v-Diffractometer.

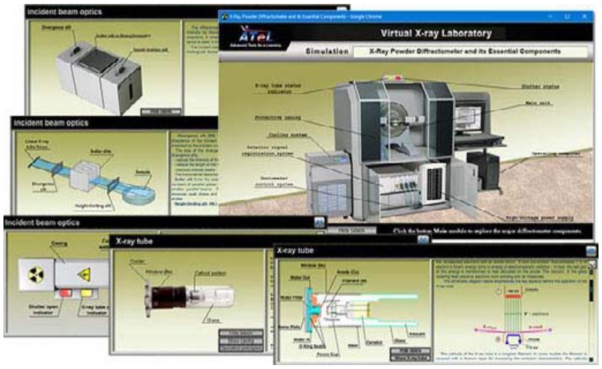

Figure 1. The Virtual Diffractometer simulation enables students to explore the design and function of an XRD powder diffractometer. A student can select any essential part (e.g. incident beam optics – top left) and virtually inspect it inside out (middle left) to better understand its operation. Screenshots on the bottom illustrate how students can examine design, major components, and basic parameters of an x-ray tube and learn the principles on which the tube's operation is based.

Virtual samples

The collection of virtual samples available for online experimentation includes alloys, ceramics, polymers, nanostructured materials, and thin films. Some samples are actual digital X-Ray patterns, the others were generated based on known crystal structure data or d-spacing and intensity (d, I) data sets.

Instructors are able to add their own virtual samples to the collection, including those simulated using the sample preparation tools associated with the v-XRLab.

Major steps of the virtual experiment

After reading the experiment description and brief theory, the student has to follow the instruction and select a sample to be investigated (See Figure 2 below.) Then, the student should virtually open the safety doors and install the sample into the holder. One of the main goals of such detailed guidelines is to help students build a mental algorithm for executing the necessary steps and required safety procedures.

At the next step, the student has to specify scanning parameters, turn on the X-ray radiation, open the shutter, and press the Start scanning button. After the scanning is completed, the generated X-ray pattern can be saved for further examination. Students can be asked to use obtained data for solving various problems.

Data obtained over the course of virtual experiments can be collected and handled manually or automatically. Virtual data can be exported to popular third-party software as well.

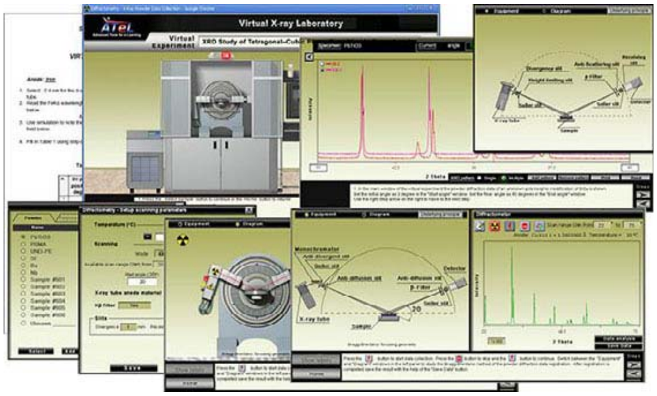

Figure 2. Screenshots of the virtual experiment "XRD Study of Tetragonal–Cubic Transition in Ferroelectrics". A sample selection form (bottom left) presents the list of available samples. The sample should be installed in a sample holder (top center). The set up form (bottom center) is used to specify parameters of scanning. The data collection interface is shown on the bottom right. The left panel dynamically displays either the goniometer status or Bragg-Brentano diagram (top right). The right panel shows the scattering X-ray pattern being recorded. The instructional panel below the simulation displays step-by-step experiment instructions for the student. The built-in utility (middle right) allows the student to measure peaks positions and intensities and compare patterns. A printed experiment worksheet is shown in the left.

USE OF v-XRLab FOR TEACHING UNDERGRADUATE AND GRADUATE COURSES

The v-XRLab has been used at five universities including the University of Maryland, University of South Florida, Massachusetts Institute of Technology (MIT), Yaroslavl State University (Russia), and Moscow State Technical University of Radio-Engineering, Electronics, and Automation (MIREA) for teaching several different undergraduate courses such as courses on materials science, crystallography, solid state chemistry, physics, solid state physics, biochemistry It has been used as follows:

1. As the only practice on the relevant subjects for students enrolled in large-scale lecture classes or in distance learning courses (See example in Figure 3);
2. For lecture demonstrations;
3. For preparing students for hands-on practice in actual X-ray labs;
4. In combination with practice using an actual X-ray diffractometer;
5. For performance-based assessment of students' ability to operate the equipment and apply gained knowledge of diffraction theory for solving practical tasks.

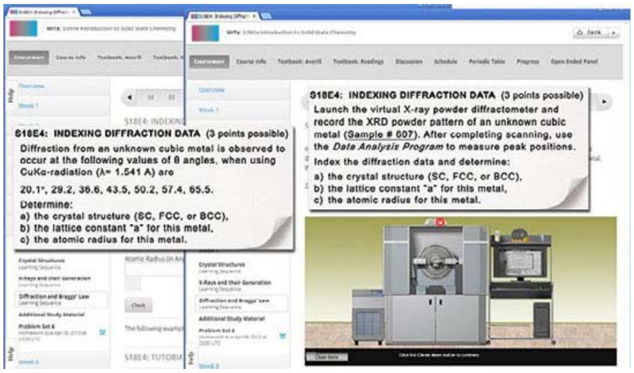

Figure 3. The screenshots of assessment pages of the undergraduate MITx course "Introduction to Solid State Chemistry" available on the MOOC edX platform. MIT Students had to determinate the crystal structure, lattice constant and atomic radius of an unknown cubic metal. Before the integration of v-XRLab (left) students were provided with the diffraction peak positions ready to be used for calculations. After the incorporating v-XRLab, students were provided with a sample number, randomly generated by the system. They had to become familiar with the equipment, perform all procedures required in the actual hands-on experiment, measure peak positions, and only after that, were they able to calculate the required parameters.

The online experiment assignments included:
Studying Bragg's Law; Determination of lattice type and constant and comparison of unit cell sizes; Indexing diffraction data and exploring the impact of x-ray wavelength and space between atomic planes on the position of diffraction peaks on a pattern; X-Ray diffraction study of order-disorder transitions in a binary alloy system and tetragonal–cubic phase transitions in ferroelectric perovskite ceramics; XRD study of the structural development of uniaxially stretched rubber; Identification of polymorphic phases of silicon dioxide (SiO_2); Qualitative phase analysis of human kidney stones using online standard reference database and reference patterns calculated from crystal structure data.

USER FEEDBACK

Students feedback

Student assessments of the online assignments using v-XRLab reveal that this e-learning tool provides excellent process visualization accompanied by a good equipment and method overview. This helped students develop a deep conceptual understanding. Students also noted that the software is user-friendly and very easy to use. Students appreciated being able to perform assignments from home at their own pace at a convenient time. This helped them master operational and maintenance skills online and prepared them for more efficient performance of a similar task in the actual x-ray laboratory.

Students also pointed out that the combination of interactive simulations with synchronized online multimedia resources associated with experiments enabled them to perform experiment tasks faster and more meaningfully. Students were interested in the opportunity provided by the cyberinfrastructure, in which the v-XRLab enables the communication with their peers from other schools and even from different countries.

Faculty feedback

According to faculty feedback, the XRLab and relevant simulations allowed them to substantially broaden their instructional palette, create educational content of a greater quality, and enhance their teaching efficacy. The v-XRLab provides instructors with the opportunity to offer students a greater number of varied exercises, challenge students with practical assignments that otherwise were difficult or even impossible to offer due to the lack of time for hands-on practice and unavailability or limited availability of physical equipment. It also became possible to expand the tasks of some experiments, e.g., to investigate phase transitions in solids over a wide range of high/low temperatures or pressures.

The modeling tools enabled instructors to prepare samples with tailored characteristics for examination of different residual stresses, textures, and crystallite sizes, offering a larger selection of crystal structures and compositions for investigation.

Faculty who taught specific crystallography courses revealed that deep exploration of design, purpose, and operation of the essential diffractometer components, such as X-ray sources, monochromators, slits, filters, detectors, etc, allowed students to better understand the impact of the scanning parameters and geometry on the positions, intensities, and shapes of the reflexes on the XRD patterns. The students were also much better at evaluating the reliability and accuracy of measured x-ray diffraction data and hence the experimental results. These instructors were also able to offer students assignments that required instant equipment reconfiguration (e.g. "replacing/changing" X-ray tubes, monochromators and detectors) and comparison data obtained at different experiment conditions.

The authoring toolkit was helpful in personalizing learning assignments and tailoring them to student backgrounds and specific educational goals and course content.

The embedded LCMS provided the option of splitting students into small collaborative groups, creating and assigning a separate task for each group or even for each individual student, and keeping track of student performance.

Based on student feedback and faculty observations, virtual experimentation enhanced students' confidence and fostered their self-reliant research capacity. They also helped students to bridge the gap between theoretical knowledge and its practical application to analyzing and comparing diffraction data.

ACKNOWLEDGMENTS

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