



Customizable Virtual X-Ray Laboratory: An Innovative Tool for Interactive Online Teaching and Learning

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Dr. Yakov E. Cherner, a Founder and President of ATEL, LLC, taught science, engineering and technology disciplines to high school, college and university students. He has extensive experience in writing curricula and developing educational software and efficient instructional strategies. Dr. Cherner introduced an innovative concept of multi-layered simulation-based conceptual teaching of science and technology. This instructional approach uses real-world objects, processes and learning situations that are familiar to students as the context for virtual science, engineering and technology investigations. He also proposed and implemented the pioneering concept of integrated adjustable virtual laboratories. To facilitate these methodologies for academic education, corporate and military training, his company developed new ground-breaking e-learning solutions, as well as relevant assessment and authoring tools. Dr. Cherner holds an MS in Experimental Physics, and Ph.D. in Physics and Materials Science. He published over 90 papers in national and international journals and made dozens presentations at various national and international conferences and workshops. Dr. Cherner has served as a Principal Investigator for several government-funded educational projects.

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Abstract: The customizable simulation-based Virtual Analytical X-ray Laboratories (v-Labs) have been developed to enable students to become familiar with the design and operation of the X-ray equipment and its major features. It allows students to gain practical skills required for conducting actual experiments and acquire the knowledge needed for collecting, analyzing and interpreting experimental data. Embedded auxiliary simulations help students learn fundamental physical principles underlying the analytical methods and equipment design in visual and interactive ways. An interactive online lesson, as well as prerecorded video lectures, animations, quizzes and other learning resources, can be called up within virtual experiments to provide “just-in-time” learning opportunities that address the educational needs of the student.

An easy-to-use authoring tool enables instructors to customize existing virtual experiments, create new ones, as well as add their own objects into the collection of accessible samples.

The v-Labs can be easily integrated with and become valuable supplements to traditional online courses on natural sciences and engineering including MOOC courses.

Introduction

The complicated and highly competitive modern engineering education requires fundamentally new concepts and novel instructional strategies in teaching and learning. As distance education rapidly grows and becomes incorporated into mainstream science and engineering curricula, truly interactive, simulation-based, online labs, which are capable of partially replacing or expanding conventional hands-on labs, are in increasing demand. The recent phenomenal popularity of engineering massive open online courses (MOOC) also prompts requests for authentic online substitutes of actual laboratory and research equipment suitable for online practices.

To push the research frontiers and educate innovators in science and engineering requires costly instrumentation, and often unique and/or custom made facilities. Even for institutions with substantial endowments, subsidizing a deficit driven by these and other costs is, in the long run, unsustainable.

Contemporary research equipment is not only extremely complex and very expensive, it is typically fully computerized. Most procedures such as calibration, data collection, data handling and interpretation are performed automatically. While this provides enormous benefits for researchers, it also creates substantial educational drawbacks, since students can access only a computer monitor and sample holder. The laboratory experimentation is reduced to installing a sample, pushing the Start button and getting the final results on the computer. All steps in between are inaccessible for students.

Virtual equipment is capable of not only overcoming this problem, but also linking the acquisition of practical skills in actual equipment operation with the learning of fundamental principles and applied methodologies underlying the corresponding experimental methods and equipment design.

Virtual X-ray Laboratories

In this research, the customizable simulation-based Virtual Analytical X-ray Laboratories (v-Labs) have been developed to enable students to become familiar with the design and operation of the X-ray equipment and its major features. The v-Labs allow students to gain practical skills required for conducting actual experiments and acquire the knowledge needed for collecting, analyzing and interpreting experimental data. Embedded auxiliary simulations help students learn fundamental physical principles underlying the analytical methods and equipment design in visual and interactive ways. The v-Labs enable students to watch and explore what is going on “under the hood” of the equipment and thus overcome the educational disadvantage of contemporary fully computerized X-ray equipment that feels like a “black box”, letting students access only a computer monitor and a sample holder.

The Virtual laboratory for studying X-ray powder diffraction and the application of the methods in materials science, chemistry, physics, geology, metallurgy, biochemistry and engineering is described and discussed below.

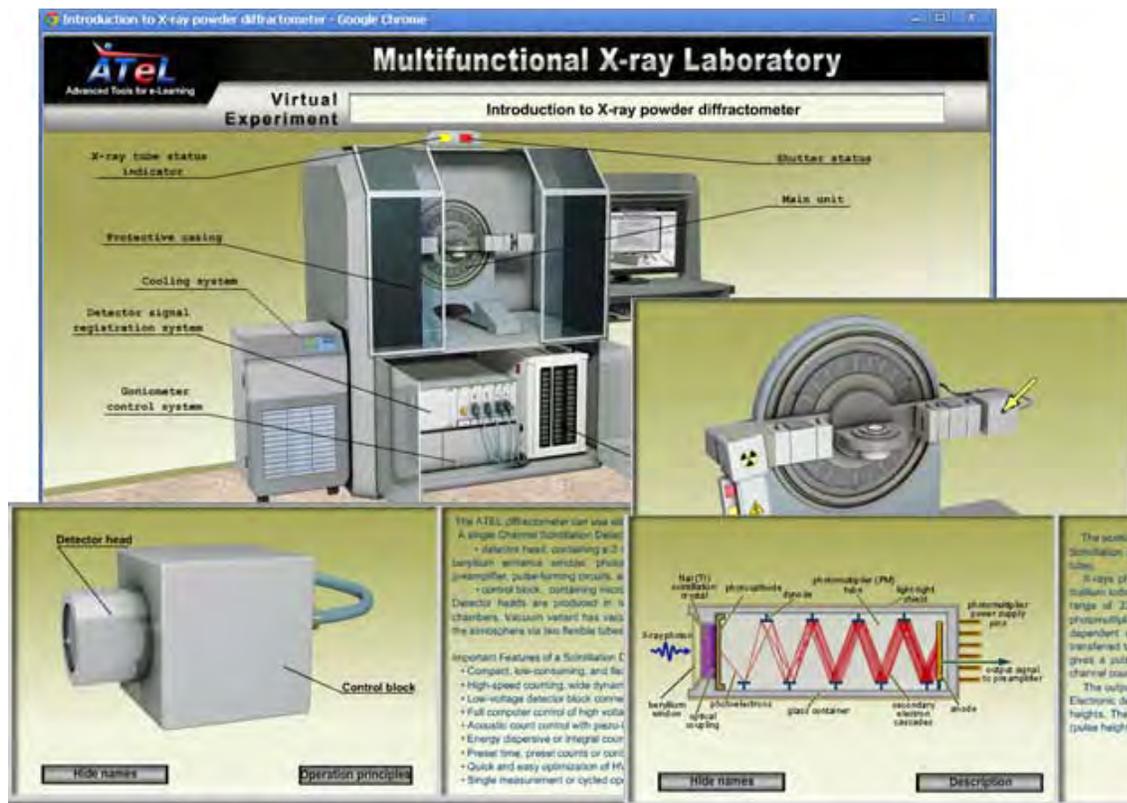


Figure. 1 Screenshots of a virtual experiment developed to introduce students to the design and functionality of an X-Ray powder diffractometer and its major parts, as well as to help them better understand relevant science laws and engineering implementations.

The learner is able to select a part (e.g., scintillation detector – bottom left) and explore in detail its design, major components, and basic parameters. Students will also learn the fundamental principles on which the part's operation is based (bottom right).

Although our virtual XRD diffractometer, which is the heart of the discussed v-Lab, does not reproduce any vendor specific instruments, it realistically imitates all major parts and devices of a fully functional diffractometer.

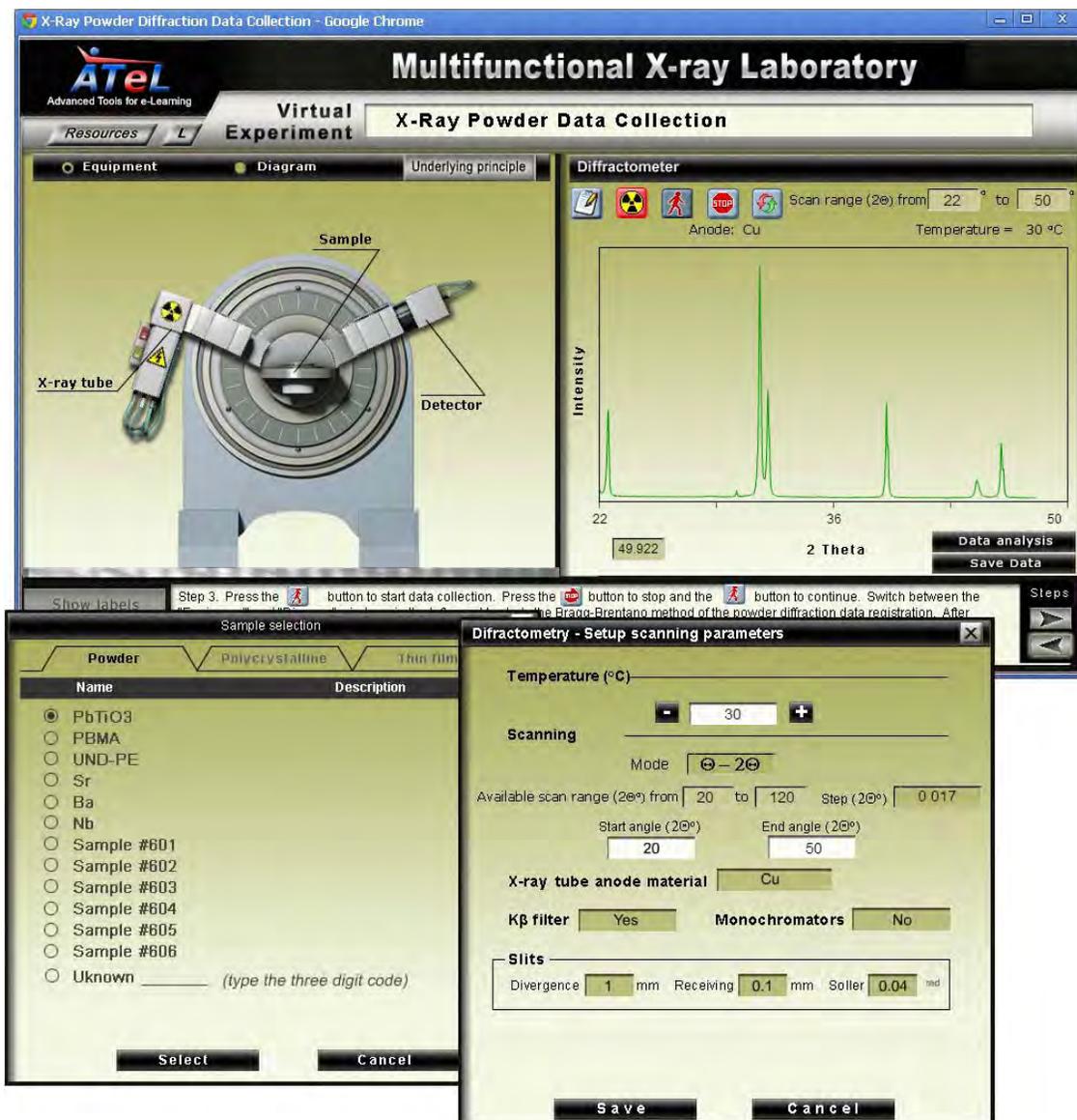


Figure 2. The screenshot in the bottom left illustrates how a student can select a sample from the open collection of samples. Then, the required scanning parameters should be specified using the set up form (bottom right). The left panel of the main experiment window (top left) dynamically presents the goniometer status, the right panel (top right) shows the scattering X-ray pattern being recorded. The instructional panel in the bottom of the main window displays step-by-step experiment instructions for the student.

Over the course of an online X-ray Powder Diffraction experiment, the student should perform all of the procedures required in an actual experiment. The virtual experiment starts with the selection of a sample to be investigated. Then, the user has to specify scanning parameters, turn on the X-ray radiation, open the shutter, and press the Start scanning button. While scanning the

specimen, the user can switch between top view of the actual setup that in real equipment is hidden under the protective cover (Fig. 2, top left) and a schematic Bragg-Brentano diagram (Fig. 3 middle left). The detailed step-by-step on-screen experiment instruction is displayed in the bottom of the interface (Fig. 2).

After the scanning is completed, the generated X-ray spectrum can be saved for further examination.

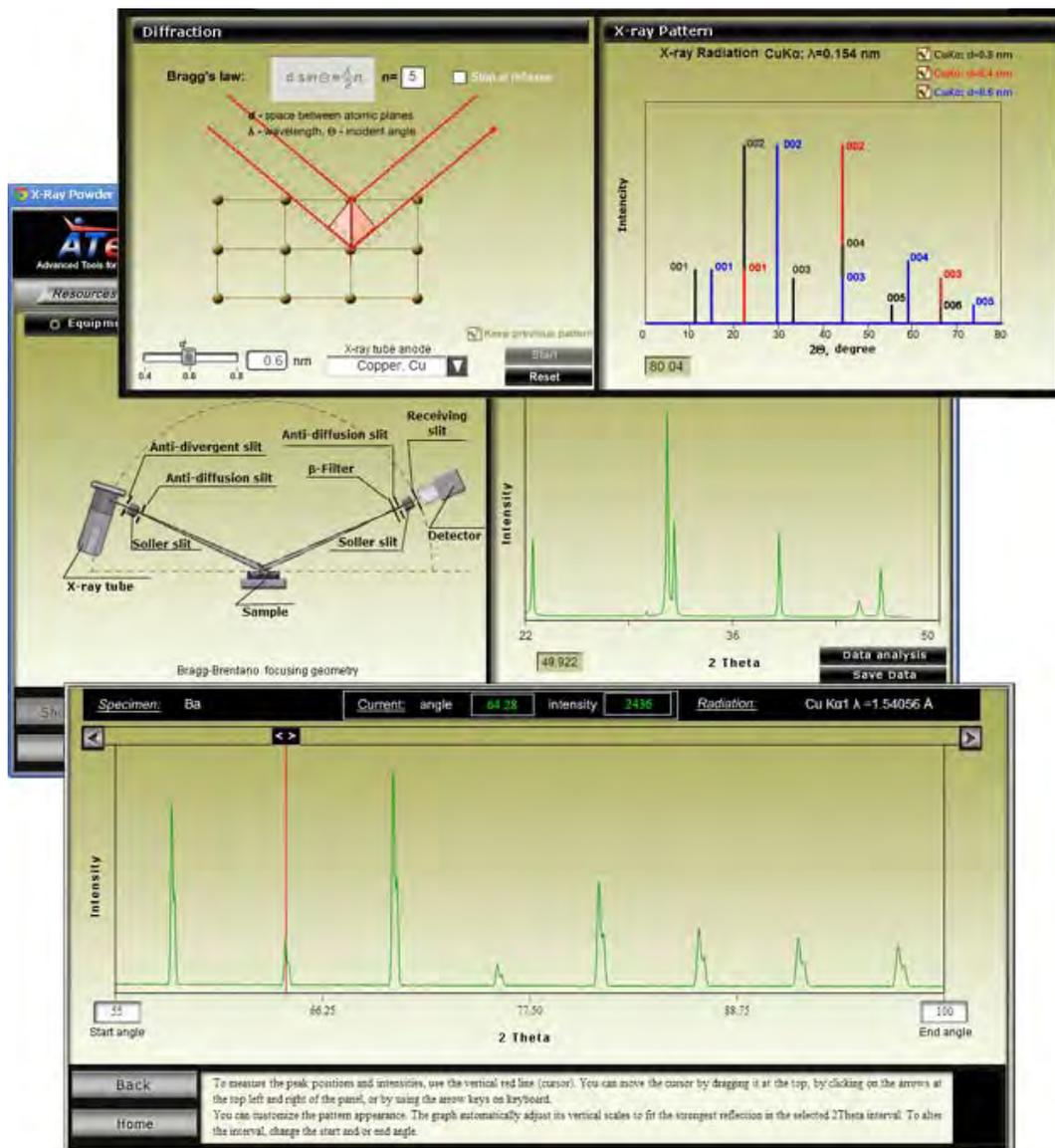


Figure 3. The screenshot at the top shows the interactive simulation that allows students to explore Bragg's law. The left panel of the main experiment window (top left) presents Bragg-Brentano focusing geometry of the diffractometer. The screenshot in the bottom presents the utility that students can use to determine the positions and intensities of the diffraction peaks.

Although all modern X-ray diffractometers are supplied with powerful software packages that can perform data analysis and most calculations automatically, it is very important to teach students how to analyze and interpret measured data, what potential causes of possible experimental errors are, and how to evaluate accuracy and reliability of the obtained results, as well as the method limitations. Virtual equipment may serve as the right tool for achieving these objectives.

The v-Lab includes software for manual data handling and analysis (Fig. 3, in the bottom).

In addition, the diffraction can also be exported in several formats compatible with variety of freely or commercially available software packages used in research labs for data analysis, calculations of structural parameters, and determination of chemical compositions.

The v-Lab also includes auxiliary simulations that visualize processes occurring inside the equipment cover and specimen. For example, the interactive Bragg's law simulation demonstrating the interaction of the X-ray beams with a crystal lattice is presented in Fig.3. Students can alter the X-ray wavelength and space between atomic planes in the crystal lattice and observe how these changes affect the positions of diffraction peaks and thus better understand diffraction of X-rays by the crystal lattice and Bragg's law.

Two major types of data are acceptable. Diffraction patterns of the first type should be obtained using an actual XRD diffractometer. All common experimental diffraction data formats are acceptable. The patterns of the second group are generated on the fly based on the known structural data of the sample.

If a calculated pattern is used, the student has the option to choose the most appropriate X-ray tube anode material and to decide whether or not to use a monochromator or $K\beta$ -filter.

The v-Lab incorporates auxiliary software for modeling the impact of a preferred crystallographic orientation or texture of polycrystalline samples, residual stresses and some other effects. Powder diffraction patterns of multiphase samples can be generated as well. The samples of chemical compounds, minerals, metals, ceramics, polymers, nanomaterials and biochemical objects can be in the form of powders, polycrystals, or thin films.

An interactive online lesson, as well as prerecorded video lectures, animations, quizzes and other learning resources, are called up within virtual experiments to provide "just-in-time" learning opportunities that address the educational needs of the student.

The v-Labs have a great potential for facilitating active online learning and transforming "e-learning by reading and watching" into a more effective "learning by doing". According to our students' feedback, this interactive and motivational way of gaining knowledge matches the learning habits of a new generation of students well.

The v-Labs can be easily integrated with and become valuable supplements to traditional online courses on natural sciences and engineering including MOOC courses available from edX, Coursera, and Udacity and other courseware providers. Fig. 4 presents the virtual experiment

associated with curriculum resources available at the web-based massive open online course (MOOC) platform edX,

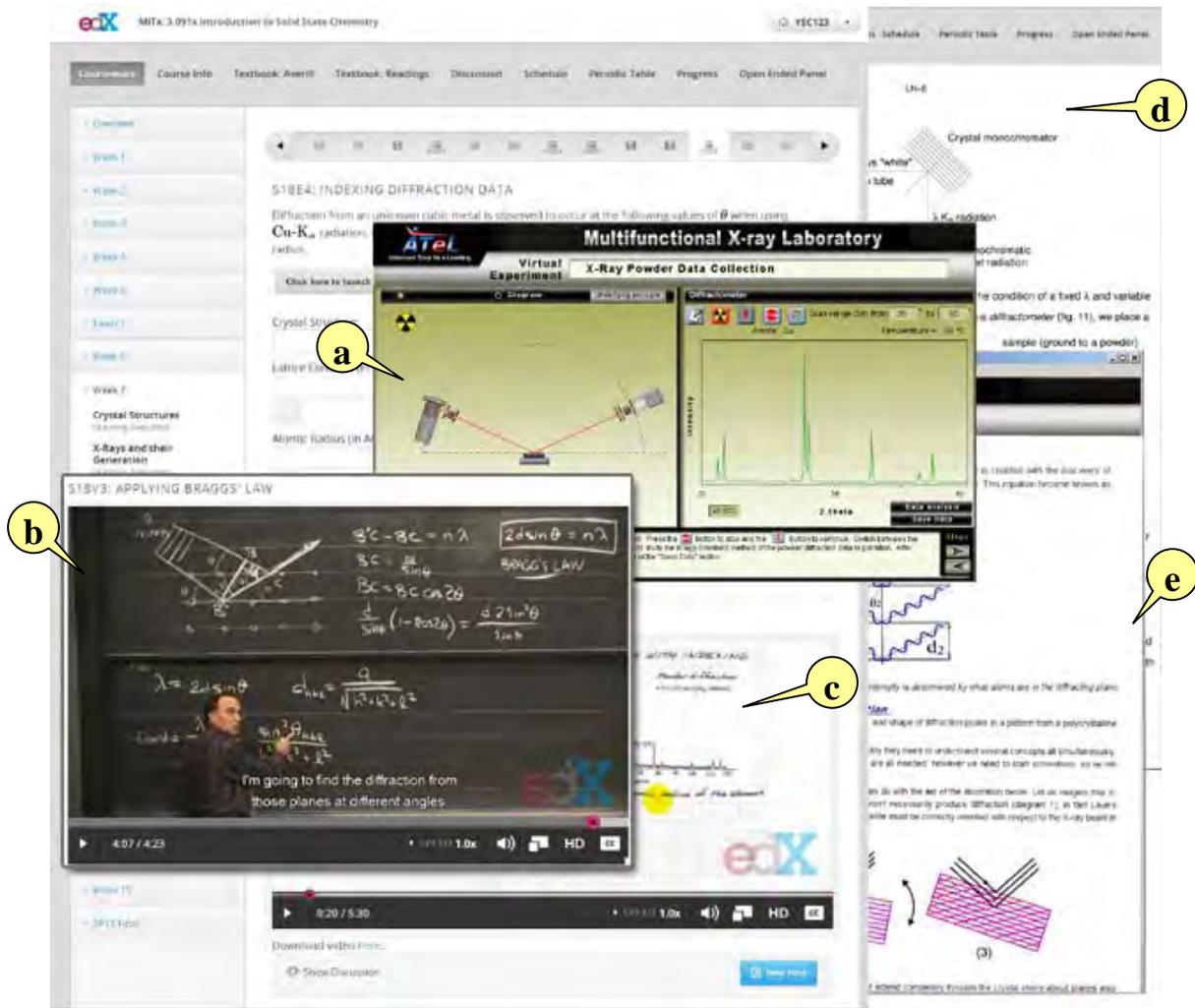


Figure 4. Virtual experiment on X-ray powder diffraction integrated with the MIT course “Introduction to Solid State Chemistry”. (a) - online XRD experiment; (b) – prerecorded lecture by MIT professor M. Cima; (c) – Prof. Cima’s animated instruction for X-ray diffraction data analysis; (d) – course textbook, (e) – interactive lesson embedded into the v-Lab.

The Use of v-Labs

Virtual labs can be integrated with student assignments. Figure 5 present an example of the homework that for evaluation purposes was offered to students of Yaroslavl State University (Russia) majoring in materials science. The students were asked to assess the online assignment using the edX platform, launch the virtual diffractometer, specify scanning parameters, and collect diffraction data, then using the obtained diffraction data, determine the unit cell parameters of a ferroelectric sample at various temperatures, find out the temperature of tetragonal-cubic phase

transition (Curie temperature), and calculate thermal expansion coefficient. Several examples of student assignments using the virtual XRD diffractometer can be found in the appendix below.

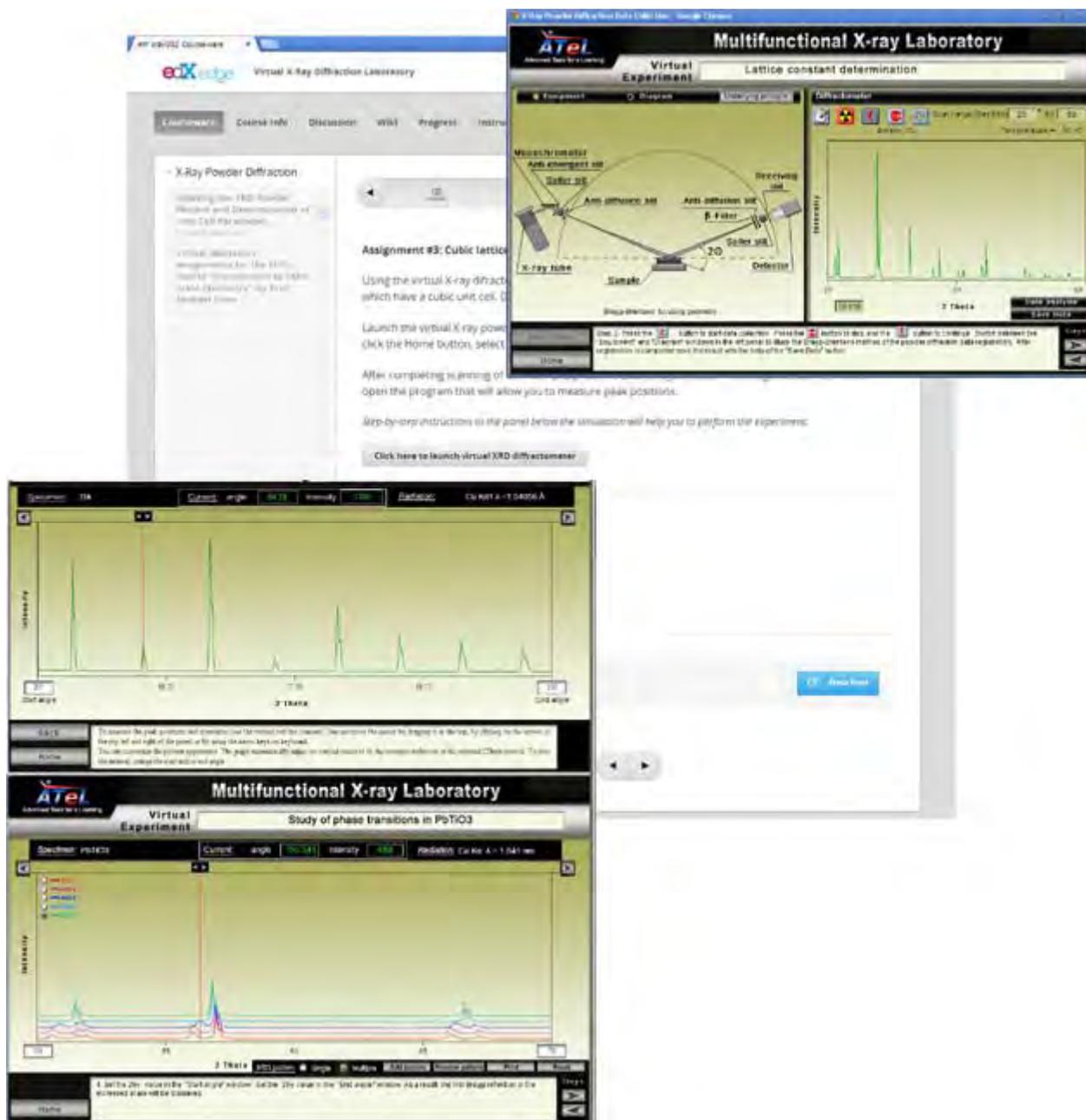


Figure 5. An example of the use of the v-Lab as a part of an assessment. In the presented test students have to use the virtual diffractometer to scan a ferroelectric sample at various temperatures, calculate the unit cell parameters and define the temperature of the phase transition (Curie point).

According to student surveys, this and similar online exercises helped them to study how to perform particular calculations, effectively learn the X-ray powder diffraction technique, and quickly grasp its application to resolving practical problems.

The v-Lab simulations can be successfully used for lecture demonstrations as well. For instance, replacing hand drawings of X-rays interactions with a crystal lattice with the Bragg's law simulations can help a lector to save time spent on drawing, to show the process dynamically, and to demonstrate the impact of various factors on the diffraction pattern.

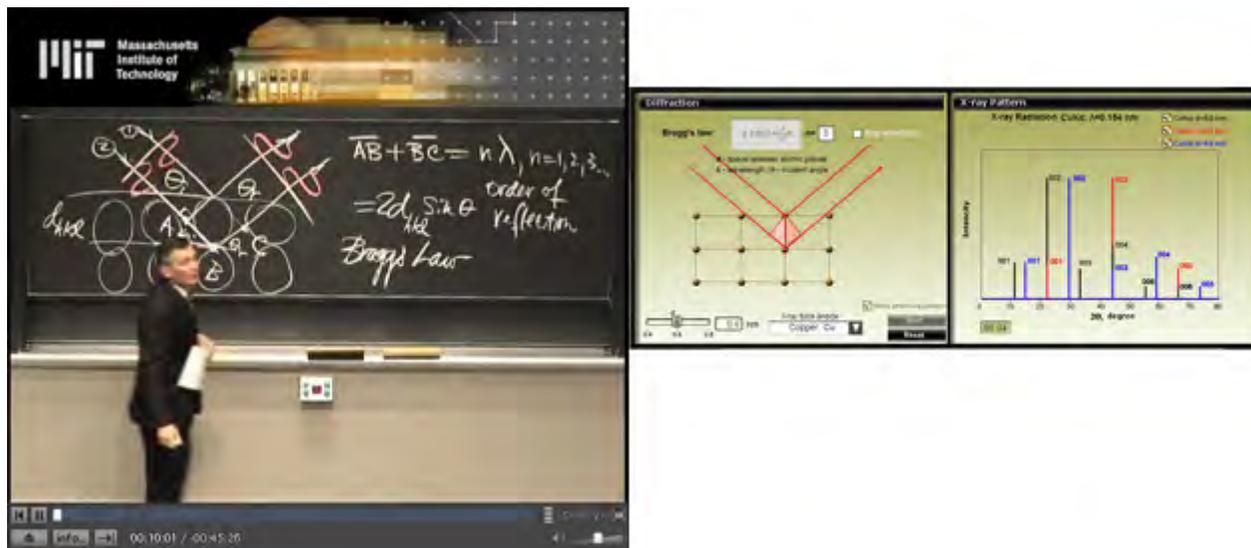


Figure 6. The video lecture on X-ray diffraction (left) available from the web-based course repository of the Massachusetts Institute of Technology (MIT OpenCourseWare) and the Bragg's law simulation (right) that can be used instead of the drawing on a black board.

Virtual experiments can potentially be combined with actual experiments and synchronized with real equipments operated either locally or remotely. Such combinations allow students and teachers to reduce practice time and demand for equipment resources and instrument time, while still acquiring hands-on experimental skills. Measured data can be compared with calculated data.

An easy-to-use authoring tool enables instructors to customize existing virtual experiments, create new ones, as well as add their own modules into the collection of accessible samples.

The v-Lab includes the utility that allows instructors to include their own samples into the open sample collection.

The v-Lab has been used as a part of homework and assessment tasks by students enrolled in large lecture classes without subsequent hands-on practice in actual X-ray labs. There were other groups of students that used the v-Lab in preparing to work with real X-ray equipment. The students' and instructors' feedback reveals that online experiments prior to actual lab practice provide an overview of the equipment and methods, and help students perform hands-on experiments with better understanding. This fact is also supported by the findings of a recent research study conducted at DeVry University in Addison, Illinois to analyze the use of computer

simulation design methods on student learning¹. The findings of the study suggest that simulation is effective when it is followed by hands-on activity to reduce the gap between theoretical knowledge and practical expertise. The instructors have also reported that highly interactive online activities using virtual equipment keeps students (users) constantly engaged and focused.

As a part of an international partnership effort, a Russian version of the v-Lab and associated resources has been created. It is currently being further developed by faculty of the Yaroslavl State University (YSU) and is used and tested by YSU students. Due to its flexibility, modules structure, and content that is focused on basic science and engineering, the v-Lab allows for simple adjustments and can be readily adapted to any US and foreign university curricula and various education systems.

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Appendix

EXAMPLES OF ONLINE ASSIGNMENTS USING THE VIRTUAL X-RAY EQUIPMENT

Experiment #1. Indexing Diffraction Data

Run the virtual X-ray diffractometer and record the XRD powder pattern of an unknown cubic metal (Sample # 607) and determine its crystal structure (enter SC, FCC, or BCC), the lattice constant, and atomic radius of the metal.

Launch the virtual X-ray powder diffractometer, select the sample #607 and obtain the XRD pattern. Use the Mo- K_{α} radiation and scan the 2θ range from 15 to 55 degrees. After completing the scanning of the sample, press the Data analysis button in the right bottom corner to open the program that will allow you to measure peak positions.

Step-by-step instructions in the panel below the simulation will help you to perform the experiment.

[Click here to launch virtual XRD diffractometer](#)

Experiment #2. Lattice type determination

The d -spacing of the (200) reflection of cubic sample #602 is 1.985 Å.

Launch the virtual X-ray powder diffractometer, select Sample #603, and obtain the XRD pattern. After completing scanning, press the Data analysis button in the right bottom corner to open the program that will allow you to measure peak positions.

Experiment #3: Cubic lattice size

Using the virtual X-ray diffractometer scan two unknown samples: Sample #602 and Sample #603, both of which have a cubic unit cell. Determine which of the samples has a larger lattice constant a .

Launch the virtual X-ray powder diffractometer, select sample #602 and obtain the XRD pattern. Then, click the Home button, select sample #605 and obtain the XRD pattern again.

After completing the scanning of each sample, press the Data analysis button in the right bottom corner to open the program that will allow you to measure peak positions.

Experiment #4: Lattice constant determination

The third XRD powder reflection of the unknown cubic sample has the Miller indices (111). Using the virtual X-ray diffractometer obtain the XRD pattern of the sample and determine its lattice constant a .

Launch the virtual X-ray powder diffractometer, select sample #602 and obtain the XRD pattern. After completing the scanning of the sample, press the Data analysis button in the right bottom corner to open the program that will allow you to measure peak positions.

Experiment #5: X-Ray Diffraction Study of Order-Disorder Transitions in CoPt System

Students have to obtain XRD patterns using the virtual X-ray diffractometer at room, distinguish superlattice vs. fundamental peaks, calculate the structure factor “F” for ordered (tetragonal) and disordered (face centered cubic) phases of CoPt, calculate order parameter “S” for all annealed samples, calculate the average particle size of ordered phase, determine the effect of the order-disorder transition on an XRD pattern and understand order-disorder transition

Experiment #6: X-ray Diffraction Study of the Structural Development of Uniaxially Stretched Rubber.

Using the virtual X-ray diffractometer students have to obtain X-ray patterns for several rubber samples, compare diffraction patterns, identify the crystalline phase occurring at high strain level and calculate unit cell parameters, perform peak profile fitting to determine percent crystallinity, verify the theoretical equation relating extension and temperature for a rubber under uniaxial stress and find any deviations from theory, and calculate cross-link density of a stretched rubber.