

## Use of a Virtual Multifunctional X-Ray Diffractometer for Teaching Science and Engineering Courses

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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. He also proposed and implemented the pioneering concept of integrated customizable online equipment and 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 100 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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Prof. Hobbs was educated at Northwestern University (BS summa cum laude, 1966) and at Oxford University (D.Phil. 1972, as a Marshall Scholar), where he afterwards held an NSF Postdoctoral Fellowship and was subsequently elected a Research Fellow of Wolfson College, Oxford. He has held professorial appointments at MIT for the last 33 years and was the inaugural holder of the John F. Elliot Chair in Materials (1992-99) there. He has served as president of the Microscopy Society of America (1987), director of the Materials Research Society (1983-86), and director of the American Ceramic Society (2003-06). At MIT, he served as Associate Chair of the MIT Faculty, chaired the faculty committees on Undergraduate Education, Curricula, Independent Activities Period, and Nominations. He also has served as longtime president of the MIT Chapter of Sigma Xi, the Scientific Research Society. He received MIT's Arthur C. Smith (a much-cherished Dean for Undergraduate Education) award for notable contributions to the Undergraduate Program. Outside the Institute, he chaired New England regional selection committees for the British Marshall Scholarships for thirteen years, the Truman Scholarships for the last six, served two years on the U.S. selection committee for Gates Cambridge Scholars, and is a member of the Advisory Board of the Council of International Exchange of Scholars (CIES-Fulbright Programs) and the Association of Marshall Scholars. He was made an Officer of the Order of the British Empire by Queen Elizabeth in 2001.

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# **Use of a Virtual Multifunctional X-Ray Diffractometer for Teaching Science and Engineering Courses**

## **Abstract**

A virtual x-ray diffractometer 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 and learn fundamental principles underlying the analytical x-ray diffraction methods. The diffractometer has been used: for lecture demonstrations, as part of homework and control assignments, for preparing students to a hands-on work in X-ray labs, in combination with actual X-ray diffractometers, and for performance-based assessment of students' ability to apply gained knowledge of diffraction theory for solving practical problems. An integrated learning management system and authoring toolkit allow instructors to design new virtual experiments and alter existing ones, create specific learning assignments for students and make learning more personal and meaningful to students.

## **Introduction**

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 a number of substantial educational drawbacks and limitations. Student laboratory task is often reduced to installing a sample and pushing the Start button. All the steps leading to final results on the computer are executed without student's involvement.

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 e-learning tools for this subject that are capable of facilitating traditional, online and blended learning, motivate students and engage them in the educational process.

To overcome these problems and provide the student with an opportunity to practice concepts, tasks, and equipment operation anytime and anywhere the virtual Multifunctional X-Ray Diffractometer (v-Diffractometer) along with associated cyber infrastructure and simulation-based interactive resources have been developed. This power and flexible educational tool can also help students to gain knowledge and practical skills that are difficult to get in using real computerized x-ray equipment. In addition, it does not require capital investment into expensive equipment during the learning process, observing rigorous safety precautions, and it does not cost anything to maintain and repair.

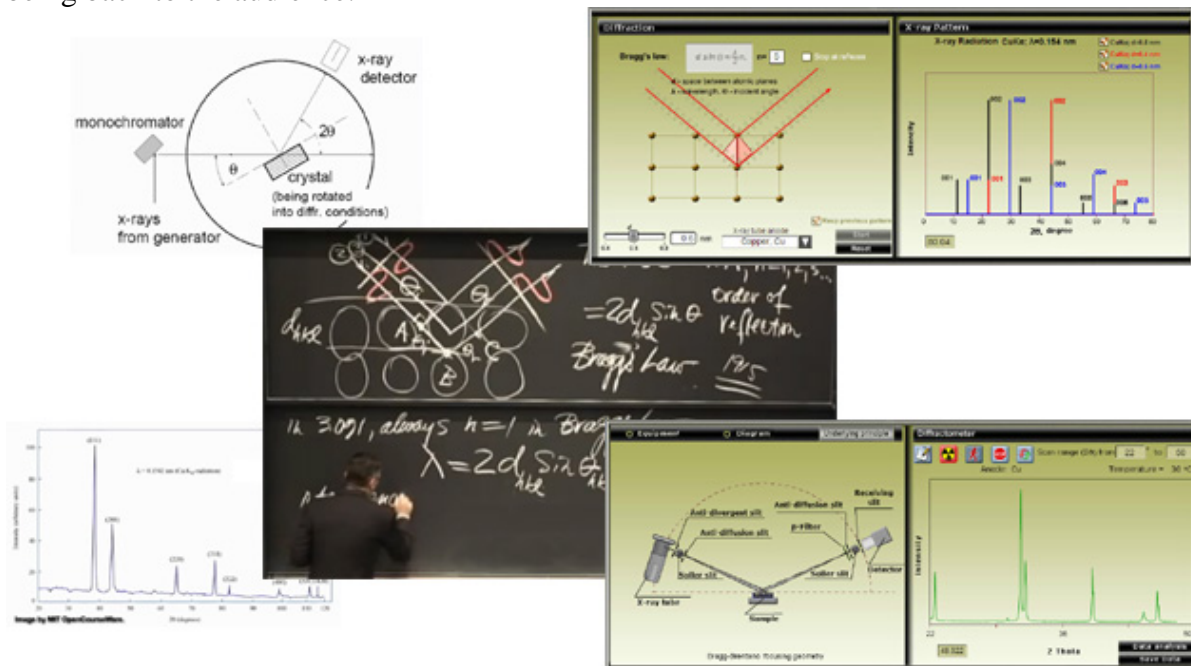
## **v-Diffractometer**

The v-Diffractometer has been implemented in several undergraduate courses on materials science, crystallography, solid state chemistry, physics, solid state physics, biochemistry and some others taught in the U.S. and Russian universities. It has been used in as follows:

1. For lecture demonstrations;

2. As the only practice on the relevant subjects for the students, enrolled in large-scale lecture classes or in distance learning courses;
3. For preparing students to 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 apply gained knowledge of diffraction theory for solving practical tasks.

Fig. 1 shows two simulations that are useful for lecture demonstrations. These simulations can replace static images and hand drawings with visual and animated Bragg-Brentano diagram and the Bragg's law simulations that allow a lecturer to improve the lectures by (i) animating the processes and presenting them in a more dynamic and attractive format, (ii) saving time spent on drawing, (iii) altering various parameters to demonstrate the impact of different factors on the positions, intensities and shapes of x-ray reflexes on an XRD pattern; (iv) minimizing time of his being back to the audience.



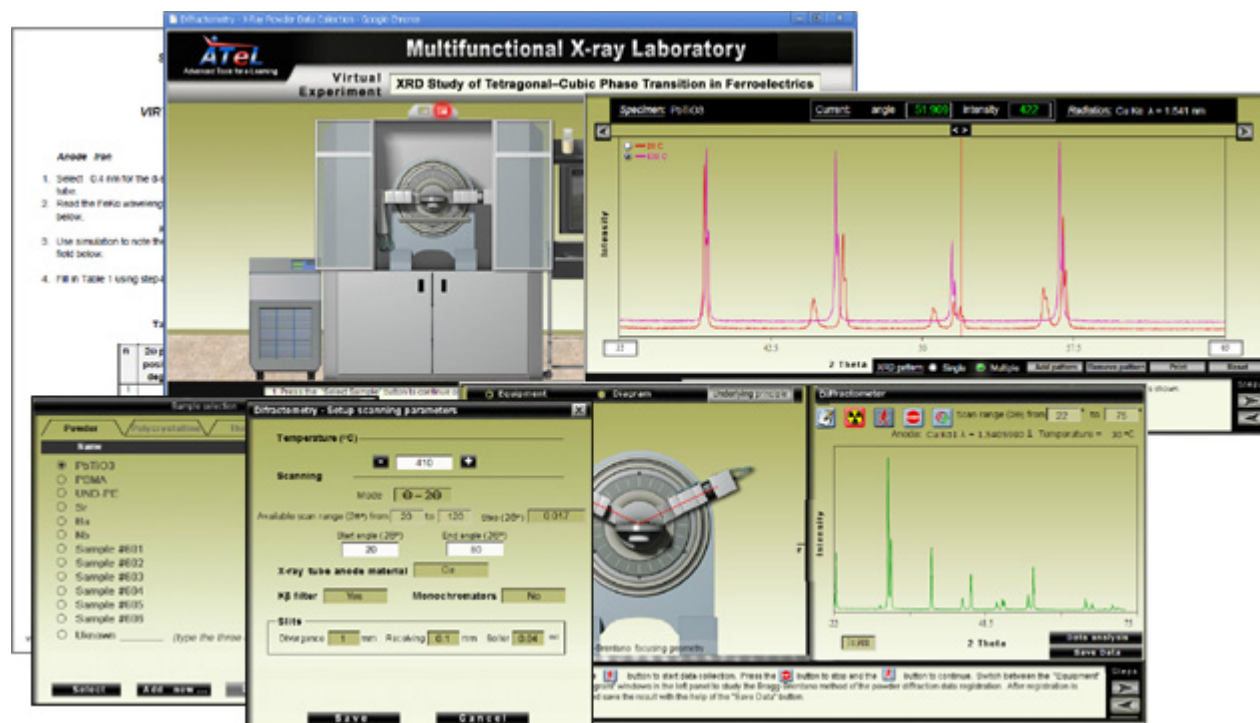
**Figure 1.** The video lecture on X-ray diffraction (in the middle) available from the web-based open course repository of the Massachusetts Institute of Technology (MIT OpenCourseWare). Two static images embedded in the lecture (on the left) and hand drawings on the black board can be replaced with interactive Bragg's law simulation (top right) and animated Bragg-Brentano diagram and dynamic diffraction pattern (bottom right).

At the present time, instructors, provide distance learners and students in large lecture classes many of whom, because of various reasons, did not have a hands-on practice in actual X-ray labs, with ready to use data for calculating unit cell parameters, indexing x-ray diffraction (XRD) reflexes, and other calculations. The v-Diffractometer makes it possible, in addition to calculations, to expose students to the XRD equipment and experiential techniques in very interactive and authentic way.

In the proposed e-learning environment, each Virtual Experiment (VE) is an integrated and self-directed online learning unit focused on a particular educational and training task. In addition to the main simulation, it includes specific learning objectives, scenario/assignment, worksheet, assessment, and, most importantly, step-by-step instructions for students. VE can also incorporate prerecorded video lectures, animations, quizzes and other learning resources that can be called up within virtual experiments to provide “just-in-time” learning opportunities that address the educational needs of the student.

Over the course of an online x-ray powder diffraction experiment, the student should perform all of the procedures required in the actual experiment. The virtual experiment begins with the selection of a sample to be investigated. Then, the student has to specify scanning parameters.

To start scanning, the student has to 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.



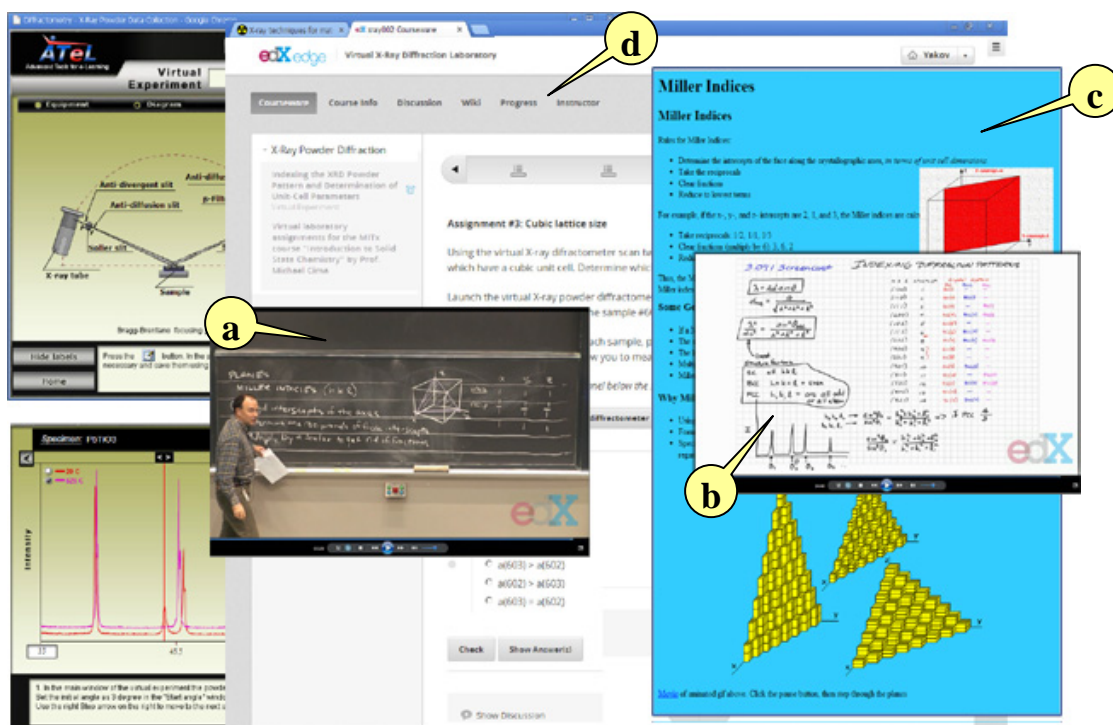
**Figure 2.** Screenshots of the virtual experiment “XRD Study of Tetragonal–Cubic Transition in Ferroelectrics”. A sample selection form (bottom left) presents the list of available samples. The sample should be installed in a sample holder (top center). The set up form (bottom center) is used to specify parameters of scanning. The data collection interface is shown in the bottom right. The left panel dynamically displays either the goniometer status or Bragg-Brentano diagram (see Fig. 1). 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 (top right) allows the student to measure peaks positions and intensities and compare patterns. A printed experiment worksheet is shown in the left.

The sample collection is open and instructors and students are able to add new samples.

The generated x-ray spectrum can be exported in several formats compatible with variety of free or commercially available software packages used in research labs for automated data analysis, calculations of structural parameters, and determination of chemical compositions. However, it is very important to teach students how to analyze and interpret measured data, identify potential causes of possible experimental errors, and how to evaluate accuracy and reliability of the obtained results, as well as the method limitations. With this in mind, v-Diffractometer incorporates software for manual data handling and analysis. Student can also print an experiment worksheet and use it for writing measured and calculated data, answering questions, etc. This makes virtual experiment even more similar to actual hands-on lab practice.

Fig. 3 below presents online resources that can be called up directly from within virtual experiments to provide students with “just-in-time” learning opportunity and address their educational needs. Any type of learning resources available in electronic format may be linked with an experiment and called up from it.

The v-Diffractometer and associated simulations can be easily integrated with and become valuable supplements to many online or traditional courses on natural sciences and engineering including web-based massive open online courses (MOOC) available from edX, Coursera, and Udacity and other courseware providers. The web page of assessment task of the edX MIT course “Introduction to Solid State Chemistry”, in which the virtual experiment has been integrated is shown in Fig. 3.



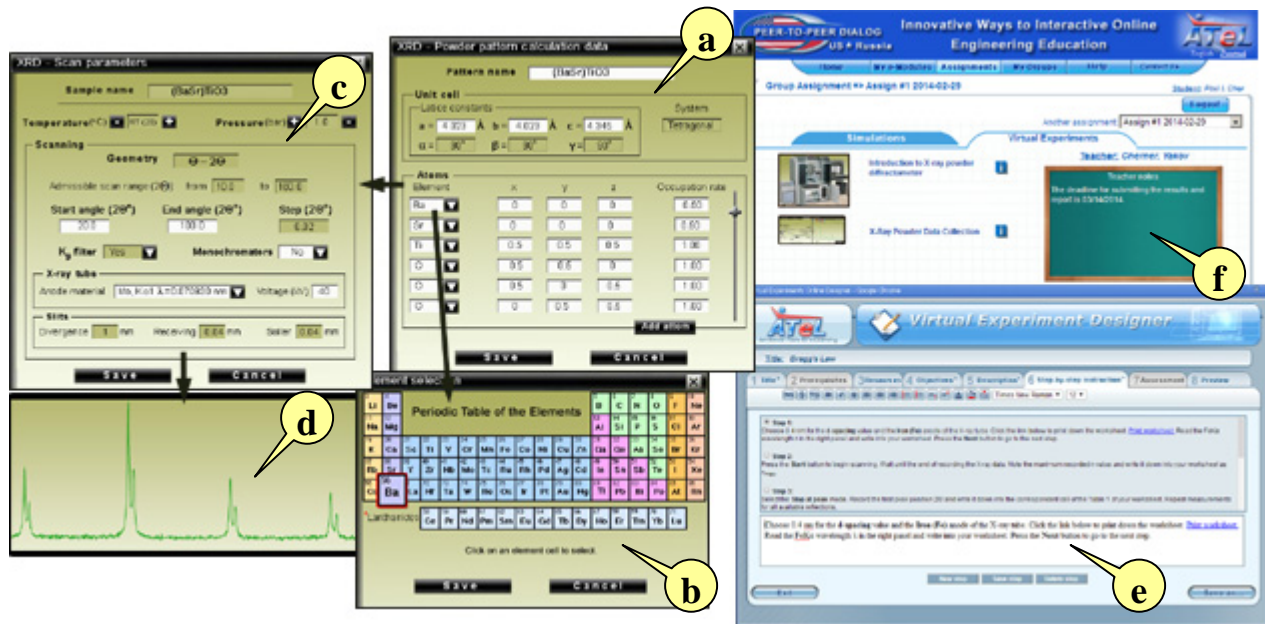
**Figure 3.** Various learning resources can be called up from within the VE including but not limited to: (a) – prerecorded lecture, (b) animated video instruction for one of the experiment tasks, and (c) online lesson. The screenshot (d) presents the assessment page of the edX MIT course “Introduction to Solid State Chemistry” in that the virtual experiment has been integrated.



The v-Diffractometer and associated programs can operate with two types of data – (1) prerecorded diffraction data of actual samples obtained using real XRD diffractometer, and (2) data simulated based on available structural information. The collection of samples available for the experiments is open and each instructor can add his /her own samples. The owner of data can decide whether the proprietary samples are available for all users or only for his or her students.

The v-Diffractometer software package used by us included modeling and authoring tools and a proprietary learning management system (LMS).

The modeling programs enable the user to prepare structural data needed for calculating XRD spectrum and dynamically simulate patterns for various states of the sample and different experiment conditions. The user is able to change lattice constants and atomic parameters, vary residual strain/stress and crystallite-size, simulate pattern for different x-ray sources, including synchrotron radiation, and for scanning with and without a monochromator. Simulated XRD data are instantly visualized and can be analyzed and compare using the package utilities. The structure data and generated patterns can be saved in a file for further analysis as well. These data can also be exported to many popular XRD analytical and modeling software packages.



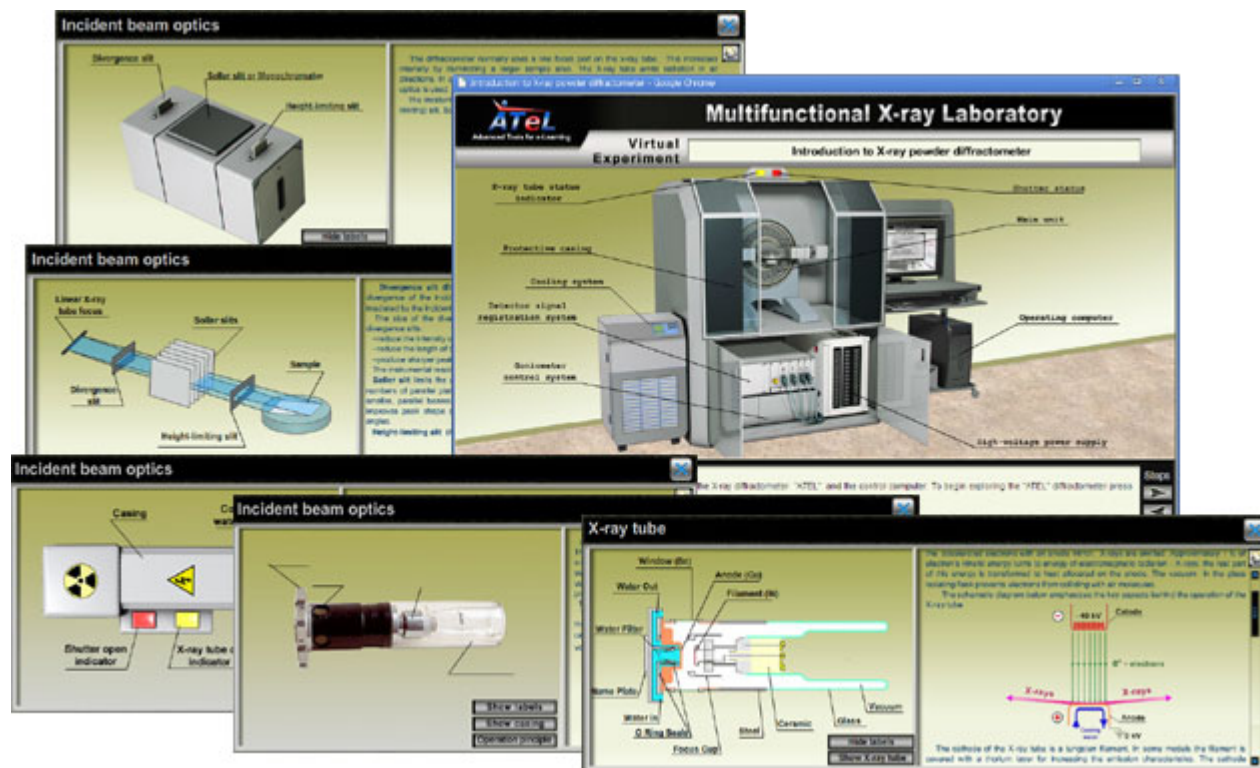
**Figure 4.** Screenshots of the modeling software (a-d), authoring tool (e) and LMS (f).

Simulation dialog forms allow the user to enter unit cell parameters and atomic coordinates (a), the Periodic Tables (b) can be brought up to select the elements. The program allows creating fully or partially vacant atomic positions, as well as positions occupied by several elements with different occupancy coefficients. The scanning set up dialog (c) requires user to enter a simulated interval, select x-ray tube anode, decide to use or not ga monochromator, crystallite size and stress. Simulated XRD powder pattern is shown in the screenshot (d).

The opportunity to vary a wide range of parameters and instantly examine the impact of these changes on XRD data and the results of experiments helps students better understand many specific features that very often remain hidden in hands-on experiments using a real diffractometer.

The v-Diffraction software package includes an authoring toolkit (Fig. 4-e) that allows instructors with no programming or scripting experience to design new virtual experiments and alter existing ones. The built-in simple LMS makes possible to split students on a small collaborative groups and create unlimited number of learning assignments for students and tailor them with student backgrounds and a specific educational goal. The instructor is able to incorporate into the VE his/her favorite resources. Hence, learning can be made more personal - and meaningful to students. The design of student assign webpage is shown in Fig. 4 (f).

The v-Diffractometer has been used as a part of homework and assessment tasks, as well as to prepare students to subsequent work with real X-ray equipment.



**Figure 5.** 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. incident beam optics – top left) and explore in detail its operation and parts (middle left). Screenshots in 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.

Although the v-Diffractometer does not exactly reproduce any vendor specific instruments, it realistically imitates all major parts and devices of a fully functional XRD powder diffractometer.

### The Use of v-Diffractometer

The v-Diffractometer has been used for teaching several different courses at five universities, including the University of Maryland, University of South Florida, Massachusetts Institute of

Technology, Yaroslavl State University (Russia), and Moscow State Technical University of Radio-Engineering, Electronics, and Automation (Russia).

The partial list of available online experiments using the v-Diffractometer included the following assignments:

- Studying Bragg's Law
- Lattice type determination
- Indexing diffraction data (exploring the impact of x-ray wavelength and space between atomic planes on the position of diffraction peaks on a pattern).
- Lattice constant determination
- Comparison of unit cell sizes
- X-Ray Diffraction study of order-disorder transitions in a binary alloy system (in this experiment students have to distinguish superlattice vs. fundamental peaks on the patterns obtained at room, calculate the structure factor "F" for ordered (tetragonal) and disordered (face centered cubic) phases of the alloy, 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.
- 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.
- X-Ray Diffraction Study of Tetragonal–Cubic Transition in a ferroelectric perovskite ceramics (students have to virtually scan a sample of a ceramics at multiple temperatures, determine the temperature of the tetragonal-cubic phase transition (Curie temperature), calculate the thermal expansion coefficient, and understand the perovskite structure and polymorphism.
- Identifying polymorphic phases of silicon dioxide (SiO<sub>2</sub>)
- Qualitative phase analysis using online standard reference database and reference patterns calculated from crystal structure data.

Such objects as ferroelectric ceramics, nanoscale thin films, metals, two-phase and three-phase chemical compounds, human kidney stones were used for virtual experimentation.

### **User feedback**

Student assessments of the online assignments using v-Diffractometer reveal that this e-learning tool provides excellent process visualization accompanied by a good equipment and methods overview. This helped students develop a deep conceptual understanding. Students also noted that the software is user-friendly and very easy to use. Students appreciate being able to perform assignments from home at their own pace at a convenient time.



Students revealed that the combination of interactive simulations with synchronized online multimedia resources associated with VEs (in particularly animations, prerecorded video lectures, interactive online lessons, prerecorded video lectures and quizzes) were very helpful for “just-in-time” focused learning subjects relevant to the performed experiment. This helps them master operational and maintenance skills online and prepare for more efficient performance of a similar task in the actual x-ray laboratory.

Students were interested in the opportunity provided by the cyberinfrastructure [associated with], in which the v-Diffractometer is incorporated to communicate with their peers from other schools and even from different countries.

According to faculty feedback, the v-Diffractometer and relevant simulations allowed them to sustainably broaden their instructional palette, create educational content of a greater quality, and enhance their teaching efficacy. Due to the use of v-Diffractometer they were able to offer students a greater number of varied exercises, challenge students with practical assignments that otherwise were difficult or even impossible to create, and expand the possible conditions of x-ray diffraction experiments.

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

Generally the lack of time for hands-on practice and unique equipment accessories does not allow students to perform experiments at non-ambient conditions. Using the v-Diffractometer students were able to explore phase transitions in solids in a wide range of high/low temperatures or pressures.

Faculty 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 better understand the impact of the scanning parameters and geometry on the positions, intensities and shapes of the reflexes on the XRD patterns, and much better evaluate the reliability and accuracy of measured x-ray diffraction data and hence the experimental results. The v-Diffractometer made possible to perform tasks that required instant equipment reconfiguration (e.g. “replacing/changing” x-ray tubes, monochromators and detectors) and compare data obtained at different experiment conditions.

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

In addition, instructors valued highly the authoring toolkit and system infrastructure including a simple built-in learning management system (LMS) that allowed them to personalize learning assignments and tailor them to student backgrounds and specific educational goals and course content. Faculty liked 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 keep track of students performance.