

Technological Innovation in Teaching and Research in Chemical Science: Development of a Computer Application for the Simulation of the Practical Works of Crystallography



Jabran Daaif, Soufiane Zerraf, Malika Tridane, Said Benmokhtar, Said Belaouad

Abstract: *The teaching-learning process has recognized a technological innovation that provides intuitive pedagogical tools for exploring new teaching strategies based on intelligent learning and computer-based virtual experiments in general science and specifically chemistry. The aim of this article is to study the educational value of interactive learning methods based on new computer and communication technologies, while applying a numerical simulation solution to the teaching of chemical experiments. Our work is based on the implementation of a computer application modeling the syntheses, structures and properties of crystallographic materials, in order to identify and study different crystalline structures proposed in theoretical courses, using a standardized set of 3D calculation and transformation functions at different angles based on mathematical calculations. To evaluate the integration of this simulation software and study its pedagogical impact on the students, the research turned to a sample of second-year students enrolled in the chemistry department of the Ben M'sik Faculty of Sciences whose the objective is to do a comparative study between the practical works of crystallography using classical methods and after numerical simulation using our computer application, in order to identify the didactic factors influencing the cognitive engagement of the learners.*

Keywords: *Chemistry, Crystallography, Modeling, Simulation, Technology*

I. INTRODUCTION

The success of the implementation of new information and communication technologies in the field of education is reflected in its most crucial role in the development of the school and university environment that offers qualitative support for the country's prosperity. The progress of these technological tools in education requires the renewal of educational systems, so that they can make learning more active and interactive more precisely in the university curriculum and offer students greater opportunities to develop their knowledge through the integration of different computer tools designed in a pedagogical framework, such as numerical and analog modeling of chemical phenomena. Researchers have found that the adoption of educational modeling and simulation software in the teaching-learning process for science subjects improves the quality of education and shapes learners' abilities to clearly imagine, understand and explain experiences. practices within the laboratory. The present work is part of the laws of crystallography that make it possible to construct, identify and study the different crystalline structures. This article aims to explore the development and pedagogical integration of a computer application that helps to carry out the practical work of geometric crystallography for different manipulations such as the identification of symmetry elements and the study of some compact and ionic structures. Our computer application works in a simple and adaptive way in the didactic norms of the chemical science, as well as the planning of the implementation of the application took into account the necessary resources [1](software of development and programming, databases, ...), funding (budgets, materials, ...), and the results of integration and evaluation. Today, there are several approaches to new information and communication technologies, including the overarching vision, underlined objectives, development planning, required facilities, learning methods and tools, and systems of the evaluation. You will find the wording of UNESCO in [2]. Our integrative approach aims to computerize the practical work of crystallography which will be detailed later.

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II. THEORETICAL CONTEXT

A. Practical works of crystallography

In the didactics of experimental sciences, practical works is a type of teaching based on practical learning with the visualization and the realization of experiments making it possible to verify and supplement the knowledge provided in the theoretical courses. This is further specified by Joris Deguet and Guillaume Piolle in [3] and by Kilien Stengel for pedagogy in teaching in [4]. The goal of crystallography practical works is to become familiar with a small number of crystalline structures and the notions of unit-cell and lattice commonly encountered in solid-state chemistry.

The session essentially consist of reading the PW to answer the questions marked in the text, to make calculations related to the theory if there are, to note the phases of experimentation and to think about representations and calculations, to discuss the results during each seance to rectify misunderstandings and obtain as much information as possible to help write the report.

1. Identification of the symmetry elements of some crystalline polyhedron and unit-cell

The purpose of this PW is to become familiar with notions of crystal symmetry at the macroscopic level using models of wooden crystals to identify the symmetry elements present. Students are led during this PW to observe, build and draw polyhedron or unit-cell to identify all types and the number of elements of symmetry that are present on the model or unit-cells studied (mirrors, axes of rotation, axes of roto-inversions and center of symmetry).

The objective of this PW is:

- Identify the symmetry elements of the proposed crystalline systems;
- Know their relative orientations;
- Find the point symmetry group and build its stereographic projection.

2. Construction and study of some compact structures

This PW consists of recognizing the three-dimensional representations of the crystals studied in progress, to study some geometric properties and to see how the atoms are stacked in a metallic crystal, as well as the parameters used to characterize these stacks:

- The coordination of one atom with respect to the other atoms constituting the stack;
- The volume of the unit-cell;
- The volume occupied by the spheres of a unit-cell in this structure;
- The relation between the unit-cell parameter a and the radius r ;
- The compactness of the structure occupied by the total spheres of the unit-cell.

We describe the model of the perfect crystal, knowing that the real crystals have defects, which give them properties. The objective of the manipulations is to study some crystalline structures deriving from a stack of compact type:

- Cubic Face-centered;
- Hexagonal compact.

3. Construction and study of some AB and AB₂ ion structures

It involves building, studying some ionic structures and calculating some important parameters based on the geometric properties of the crystals studied in progress. The aim of this PW is to study some ionic structures of types AB and types AB₂.

The ionic structures proposed in the manipulations are summarized in the following table:

Table- I: Ionic structures proposed in the manipulations of the third PW

| | | | | |
|--------------------------------------|---------------------------|---------------------------------|-------------------------|----------------------|
| AB type structure | NaCl | ZnS Blende | ZnS wurzite | NiAs Nickel Arsenate |
| AB₂ type structure | CaF ₂ fluorine | CdI ₂ cadmium iodide | Rutile TiO ₂ | |

The objectives of the different manipulations are:

- Look on the different unit-cell octahedral sites;
- Count the number of octahedral sites;
- Position the ions;
- Find the coordination of each of the ions;
- Establish the relationship between the unit-cell parameter a and the rays;
- Find the number of forms grouping by unit-cell;
- Calculate the density of the crystal;
- Give the reduced coordinates of each ion;
- Draw in perspective the polyhedron formed by the ions.

B. Numerical modeling of practical work

1. Modeling and computer simulations

Numerical modeling is one of the most used simulation methods in chemical practice during PW sessions, to represent a system by another, easier to understand. In our study this process is also used to attend all sorts of didactic constraints to the virtual projection of different crystallographic elements (polyhedron, structures and crystalline unit-cells) by providing a learning environment as support of:

- Visualization of crystalline structures in three dimensions;
- Identification of the parameters and characteristics of the unit-cells;
- Representation of the data and their interpretations;
- Collaboration of information for discussion and scientific argumentation.

Such an analog modeling consists of constructing a crystallographic system that reproduces more or less a phenomenon that one wishes to study [5]. The observation of the behavior of the model makes it possible to draw lessons on the phenomenon of interest.

We present in the following figure the process of the modeling starting from the real system to the computer system:



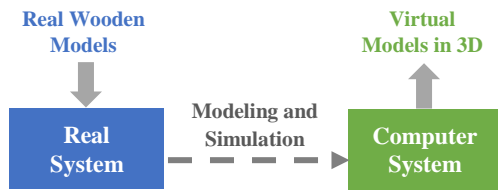


Fig. 1. Modeling process by the computer application

2. Didactic principles

From a didactic point of view, the theoretical knowledge given in course is supplemented by an apprenticeship in practical methods, taking into account that the learner's thought and imagination is not virgin and is not a passive receiver of knowledge which would be given by the teacher [6].

We can define the objectives of various tools and pedagogical means presented to the laboratory in the PW session for practical experiments:

- Understanding of the theory;
- Learning manipulation techniques;
- Learning the scientific process;
- Motivation of students.

Based on these objectives we can present wooden models as geometric shapes carved on wood to learn to recognize the morphology of crystals. They have a considerable didactic value in crystallography for the determination of symmetry elements in crystals. The proposed wooden models represent some coordination polyhedronas well as the primitive forms of the seven crystalline systems.

Our modeling computer application saves time spent in wood-based manipulations in the laboratory where students can visualize the crystalline structures in three dimensions and identify different parameters and discuss group information with the teacher on the platform developed in our computer tool.

III. METHODOLOGIE

The access to numerical modeling tools for the practical works of crystallography is done through simulation software that creates a favorable virtual environment for a good cognitive engagement of students who often cannot use certain instruments in the real laboratory within the limit of materials used in practical experiments (wooden models).

A. Analysis and specification

The aim is to develop a computer application for educational use whose purpose is to create three-dimensional representations of different crystalline structures that we want to visualize and study, they are defined in their three dimensions and they can thus be exposed from different angles. It is a new technical tool that allows modeling the stacks, calculating the coordinates, the volume, and the compactness of the different unit-cells. The application also allows to visualize the different octahedral and tetrahedral sites based on the animated representation in three dimensions.

A graphical interface of the application allows the student to create crystalline structures and study the reduced coordinates of atoms in a unit-cell and perform the

manipulations explained previously by answering the questions prepared by the teacher to generate files representing the results after authentication to access the system.

The following figure shows the first page that appears to describe the purpose of each of the crystallography module's practical work:

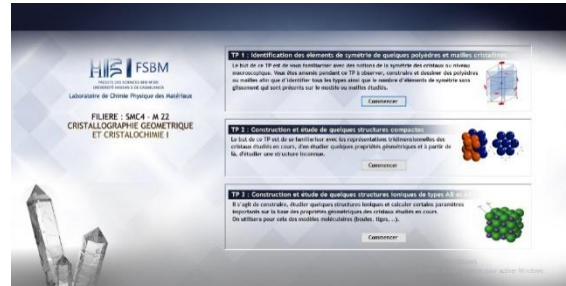


Fig. 2. The first page of the application to access the PW

B. Design and development architecture

The design of an educational simulation software is a process that aims to formalize all the preliminary stages of the development of a system to make it more faithful to the needs of the user [7].

The design and development of the application developed in this work will follow three major phases:

Table- II: Steps of realization and integration of the application

| | |
|---|---|
| Functional Analysis and Specification of the problem | The specification of the problem of manipulations is a preliminary step, in which the functional needs of each PW are studied in relation to didactical constraints and from a pedagogical point of view. In this phase, we study the modeling techniques as well as the architecture of the application. |
| Development and programming | The installation of the programming tools (work environment, database), the programming of the application and the tests to be performed are carried out in this part. |
| Integration and evaluation | This phase concerns the educational integration of the simulation application, where the user (the student) accesses the virtual environment of the PW and performs the manipulations under a teacher's supervision. |

C. 3D modeling computer tools

The action of modeling in 3D is, in a way, the three-dimensional representation of the objects that one wishes to visualize; in our case it is crystal structures and unit-cells. The modeling tools can be simple geometrical transformations, or can realize more complex transformations (assembly, texture, color, ...).

The programming of our three-dimensional modeling algorithm was based on graphically powerful technical tools allowing to model the shapes of our structures according to the different crystalline systems, and which are:

- Cubic;
- Quadratic;
- Hexagonal;
- Trigonal;
- Orthorhombic;
- Monoclinic;
- Triclinic.



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We chose to work with a set of 3D image calculation functions (OpenGL) and numerical calculation methods (Euler Algorithm).

1. OpenGL (Open Graphics Library)

It is a very complete graphical library that is available on many platforms (in our case the Framework.Net) and makes it possible to develop 2D and 3D applications quite easily. It allows a program to declare the geometry of objects as points, vectors, polygons, bitmaps, and textures. OpenGL performs projection calculations to determine the image on the screen, taking into account distance, orientation, shadows, transparency and framing. You can refer to [8,9].

The following figure shows the three-dimensional representation of a cubic system using the OpenGL library:

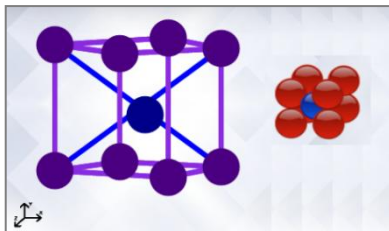


Fig. 3.Centered cubic system

We can find in OpenGL:

- Homogeneous matrices for 3D coordinate projection;
- Graphical primitives (points, lines, triangles ...);
- Image primitives Buffers (image, Z-buffer, ...);
- Optimization functions;
- Higher level libraries that simplify the use of primitives.

The OpenGL library has many features, which allows our application:

- 3D rotation of unit-cells;
- Filling by atoms;
- Detection of symmetry elements;
- Detection of octahedral and tetrahedral sites;
- The detection of reduced coordinates.

2. Algorithm based on Euler matrices

The movement of a solid relative to a reference system involves six parameters, which are the three coordinates describing the position of its center of mass (or of any point of the solid) and three angles, called the angles of Euler. Euler angles can be used to represent the orientation of each crystalline structure with respect to a fixed landmark.

In a 3-dimensional Euclidean space, the rotation matrices correspond to the rotations of the crystal structures around the x, y and z axes (respectively) used in our application are:

$$R_x(\theta) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \theta & -\sin \theta \\ 0 & \sin \theta & \cos \theta \end{pmatrix} \quad (1)$$

$$R_y(\theta) = \begin{pmatrix} \cos \theta & 0 & \sin \theta \\ 0 & 1 & 0 \\ -\sin \theta & 0 & \cos \theta \end{pmatrix} \quad (2)$$

$$R_z(\theta) = \begin{pmatrix} \cos \theta & -\sin \theta & 0 \\ \sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (3)$$

The goal of this method is to make rotations of all

crystalline systems after construction and visualization.

The following figure shows an interface that shows the simple cubic, centered cubic, face centered cubic, and compact hexagonal systems, and a second figure presenting the identification of the crystalline parameters of the cubic system as well as the access to the manipulation to answer the questions:

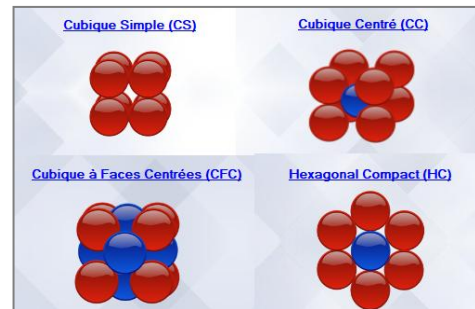


Fig. 4.Examples of crystalline structures

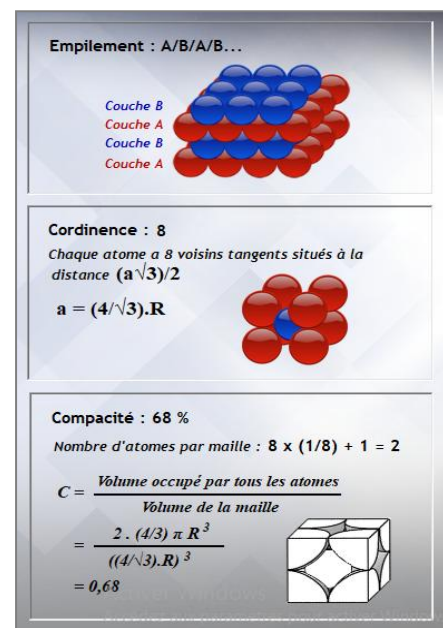


Fig. 5.Crystalline parameters of the centered cubic system

The verification of our models is intended to test and ensure that the modeling have been correctly developed and thus aims at the same time the capabilities of the application.

The algorithm developed in this work is a process to follow to carry out the steps of the practical work:

For the first experience:

- 1) Choose a crystalline system;
- 2) Construct a polyhedron in 3D;
- 3) Identify the elements of symmetry; (mirrors, axes of rotation, axes of roto-inversions and center of symmetry);
- 4) Detect relative orientations;
- 5) Detect point symmetry group;
- 6) Build the stereographic projection.

For the first experience:

- 1) Identify the coordination of an atom with respect to the other atoms constituting the stack;
- 2) Identify the volume of the unit cell;
- 3) Identify the volume occupied by the spheres of a unit cell in this structure;
- 4) Calculate the relationship between the unit parameter and the radius r ;
- 5) Calculate The compactness of the structure occupied by all the spheres of the unit-cell.

For the third experiment:

- 1) Detect the different octahedral and tetrahedral sites;
- 2) Count the number of octahedral sites;
- 3) Position the ions ;
- 4) Find the coordination of each of the ions;
- 5) Find the number of forms grouped by unit cell;
- 6) Calculate the density of the crystal;
- 7) Give the reduced coordinates of each ion;
- 8) Draw in perspective the polyhedron formed by the ions.

IV. EVALUATION AND EXPERIENCE

To evaluate the success rate of the integration of our modeling application, the second year (semester 4) students enrolled in the Ben M'sik faculty of sciences performed the three manipulations of the crystallography module in the laboratory of physical chemistry of materials.

The goal is to deduce teachers 'perceptions of interactive classroom learning methods and students' interpretation of results.

For each practical manipulation, the interfaces presented by the software make it possible to do different experiments: creation, tracing, identification, calculation, ...

A. PW1: Identification of the symmetry elements of some crystalline polyhedron and unit-cell

The steps a student can follow to achieve this manipulation are:

- Detect in 3D structures the elements of symmetry;
- Identify their relative orientations in the same interface;
- Build your stereographic projection based on the coordinates shown in the figure.

B. PW2: Construction and study of some compact structures

Visualize the stacks in 3D to find: The coordination, the volume of the unit-cell, the volume occupied by the spheres, the relation between the parameters of the unit-cells, the compactness.

C. PW3: Construction and study of some AB and AB2 ion structures

The steps a student can take to complete this third experience are:

- Search 3D unit-cells for octahedral sites;
- Position ions on three-dimensional representations;
- Detect the coordination of each of the ions;
- Calculate the density of the crystal;
- Calculate the reduced coordinates of each ion in the same interface;

- Draw graphically on a graphical interface the polyhedron formed by the ions.

V. RESULTS AND DISCUSSION

We selected in our study a sample of 200 students to interview and establish diagnostic tests and survey questionnaires in order to make a comparative study between classic methods using the material that is in the laboratory (wooden models), and the modeling method based on the computer application. The students are divided into two groups (each group contains 100 students), the first performed the manipulations in a classic way based on the wooden models. The second group used the computer application as a simulation tool that creates a virtual laboratory where the students could carry out all the manipulations by studying the different crystalline structures.

The same diagnostic tests scored out of 20 are represented in both groups include questions about the content of each manipulation; visualization, design, identification and calculation of parameters and we realized a questionnaire for the teachers on the pedagogical practice on computer, the time resulting during the sessions of the PW, the availability of the virtual objects in the application, and the digital generation of the results . A second questionnaire for the students includes questions of satisfaction on the improvement of the understanding of the practical manipulations of crystallography and the communication with the new virtual environment represented by our software solution within the laboratory.

According to the statistics of the diagnostic tests collected for each PW, 89.20% of the students who worked on the three manipulations by the computer method using the simulation application had a note above 15/20 compared to the students of the other group who worked by the classical methods 50.27% could have a note higher than 15/20. We chose the note of 15/20 as the threshold for comparing the classical method and the technological method.

We present in the following table the percentages of the students who had more than 15/20 for each PW:

Table- III: Percentages of students who scored above 15/20

| | Group 1 | Group 2 |
|------------------------------|---------|---------|
| First Practical Work | 33.41% | 79.99% |
| Second Practical Work | 56% | 89.86% |
| Third Practical Work | 61.40% | 97.76% |
| Total Result | 50.27% | 89.20% |

We scheduled a PW session for first group students who worked through the classical method to redo the three manipulations using the new method of modeling and another diagnostic test was prepared to the teachers to evaluate the pedagogical impacts of using the technology tool on students.

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We found that the majority of students had a score above 15/20, as shown in the table IV, which seems effective for students who have tried to interact with PW to understand the phenomena of crystallography by a virtual simulation on a computer.

Table- IV: Total number of students scoring above and below 15/20

| | Students with a note greater than 15/20 | Students with a note below 15/20 |
|--------------------|---|----------------------------------|
| Number of students | 90 | 10 |
| percentages | 90,22% | 9,78% |

The following chart shows the percentages of students in the first group before and after using our computer application:

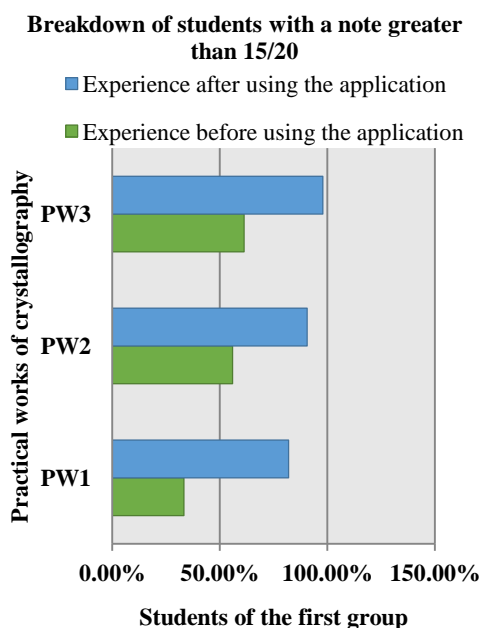


Fig. 6. Percentages of students in the first group with a note above 15/20

The questionnaire survey that we did is an important step in our study that allows for a survey of student satisfaction and interaction with the new technological environment, and a second questionnaire for teachers to assess the impact of the educational integration of our application.

The questionnaire deals with:

- Conditions of use (Relation with the course, time, number of students, material);
- Scientific content (Prerequisites, objectives, results, evaluation);
- Educational interest (skills development).

The results have been favorable and go to achieve the educational objectives recommended for an effective integration of this computer system. The following two figures illustrate the percentages of satisfaction for the students and the success rate of the pedagogical integration of the computer tool:

Percentages of satisfaction

- Disagreement 2 %
- Rather disagree 6%
- Rather agree 22%
- D'accord 70%

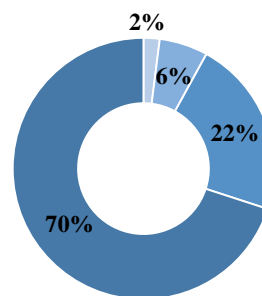


Fig. 7. Satisfaction questionnaire result of the first group of students

Levels of Success of Application Usage

- No High 4%
- High 22%
- Very High 74%

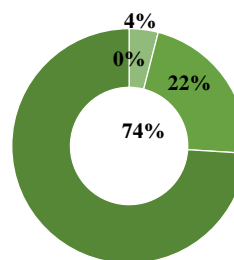


Fig. 8. Success rate of use of the computer application

In order to guarantee a fluent communication with the students, the teachers who followed the phases of this study mentioned that this new computer tool is beneficial at the pedagogical level and such a simulation and modeling process allowed us to reach the educational objectives of the students.

VI. CONCLUSION

With regard to innovation in the new information and communication technologies, adopting a new teaching mode based on digital resources is a substantial part of the university curriculum, which led us to study the Pedagogical integration of technological tools in the teaching of chemistry and to set up a computer application allowing the simulation of the practical works of crystallography in the laboratory of physical chemistry of materials within the Faculty of Sciences Ben M'Sik. The new virtual reality lab is presented using a graphical platform developed using a set of three-dimensional computational functions provided by OpenGL which is included in the .Net framework, as well as a set of mathematical functions and arithmetic calculation based on Euler's laws allowing students to orient the different crystalline structures and to identify different parameters and crystallographic characteristics.

Our computer solution was benevolent at the pedagogical level according to the survey conducted to chemistry students enrolled in the second year; the statistics were favorable goes to the goal of this work to optimize and rehabilitate teaching-learning practices in a didactic context.

The motivation to continue the integration of new technological tools will lead us to study other practical chemistry-physics work for a better integration of simulation and modeling applications.

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