Pedagogical engineering to the teaching of the practical experiments of chemistry: Development of an application of three-dimensional digital modelling of crystalline structures

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Abstract: Technological innovation in science provides complementary tools for exploring new teaching strategies within a pedagogical framework that promotes interaction between the teacher and the learner. This work is based on the implementation of a computer application modeling crystallographic material structures, in order to identify and study the different crystalline structures and their characteristics, based on the techniques of three-dimensional modeling covering the OpenGL library and the Euler rotation matrices, and developed by the C# programming language. The analysis and design of this study ranging from the study of the existing, the identification of the problematic, modeling and development, and finally the validation tests. Our research is aimed at second-year chemistry students at Ben M’sik Faculty of Science, Hassan II University of Casablanca, Morocco. We wish to conduct a comparative study between classical methods and after numerical simulation, in order to identify didactic factors influencing the cognitive engagement of the learners.
engagement of learners. The results were good, 89.20% of students in the first
group who worked on manipulations using the simulation application scored above
15/20, and 90.22% scored above 15.20/20 for the second group after completion of
the manipulations according to the two modalities (traditional and computer).
Teachers mentioned that the results have been favorable and support the recom-
mended educational objectives for effective integration of this computer system,
which seems to be effective for students who have tried to interact with the
practical work to understand the phenomenon of crystallography by a virtual
simulation on computer.

Subjects: Computer Science; Engineering & Technology; Education; Information Science
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1. 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 differ-
ent computer tools designed in a pedagogical framework, such as numerical and analogy model-
ling 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. Different ionic struc-
tures, for example, have been proposed in different manipulations, as shown in table 1
below.

Technological innovation in education provides process simulation software and design services
in the chemical, oil, gas, pharmaceutical, energy or other process industries in the scientific world.
For example, there are software programs that simulate the kinetics of a chemical reaction over
time and highlights some factors and properties for intelligent study of different reactions. There
are thus two-dimensional and three-dimensional modeling and tracing applications of curves
representing nanoscopic chemical and characteristic properties.

We quote for example:

- Avogadro: a chemical structure editor for drawing a three-dimensional molecular composition,
  with several angles and perspectives.
- Origin: scientific data processing and analysis software for drawing 2D and 3D graphs
- Wien2k: software for performing quantum calculations on periodic solids

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 develop-
ment and pedagogical integration of a computer application that helps to carry out the
practical work of geometric crystallography for different manipulations such as the identifica-
tion of symmetry elements and the study of some compact and ionic structures. Our com-
puter 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 (software of development and programming, databases, ...), funding
(budgets, materials, ...), and the results of integration and evaluation (Munir, 2010).
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. This is in line with the wording of UNESCO (Khvilon, Evgeni, Patru, Mariana, UNESCO, 2006). Our integrative approach aims to computerize the practical work of crystallography which will be detailed later.

2. Theoretical context and literature review

2.1. 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 (Deguet & Piolle, 2007/2008; Stengel, 2008).

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.

Practical work sessions consist mainly of:

- Read the practical work to answer the questions indicated in the text;
- Perform calculations in relation to the theory;
- Note the phases of experimentation;
- Reflect on representations and calculations;
- Discuss the results at each session;
- Correct misunderstandings and get as much information as possible to help in writing the report.

2.1.1. Identification of the symmetry elements of some crystalline polyhedral and unit-cell

The purpose of this practical work 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 practical work to observe, build and draw polyhedral 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) (Said, Benmokhtar, & Omar, 2017/2018).

The objective of this practical work is:

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

2.1.2. Construction and study of some compact structures

This practical work 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 (Said et al., 2017/2018):

- 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 compacte.

2.1.3. Construction and study of some $AB$ and $AB_2$ ion structures

In this part we will work by the ions, so an ion is an atom or a molecule carrying an electric charge, because its number of electrons is different from its number of protons. There are two main categories of ions: positively charged cations, and negatively charged anions.

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 practical work is to study some ionic structures of types $AB$ and types $AB_2$ [5]. Such as sodium chloride which is an ionic chemical compound of formula $NaCl$. Calcium fluoride is an inorganic compound of formula $CaF_2$. This ionic compound consisting of calcium and fluorine is naturally present in nature in the form of fluorine (also known as fluorite).

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

| AB type structure | NaCl | ZnS Blende | ZnS wurzite | NiAs Nickel Arsenate |
|-------------------|------|------------|-------------|---------------------|
| AB2 type structure | CaF$_2$ fluorine | Cd$_2$ cadmium iodide | Rutile TiO$_2$ |
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 (Sciences Modélisation, ). The observation of the behavior of the model makes it possible to draw lessons on the phenomenon of interest.

We present in the Figure 1 the process of the modeling starting from the real system to the computer system:

2.2.2. 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 (Leslie & Gale, 2012; Piaget, 1937).

We can define the objectives of various tools and pedagogical means presented to the laboratory in the practical work 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 polyhedra as 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.

3. Methodology
The access to numerical modeling tools for the practical work of crystallography is done through simulation software that creates a favorable virtual environment for a good cognitive engagement of students.
The first step of such a study procedure is the analysis of the existing and the problematic, for this we have led to a research on the tools used in the rooms of the practical work (wooden and plastic models), the theoretical course materials, as well as the didactic transposition within the practical experiments sessions of the crystallography module. We conducted an analysis at the pedagogical level through meetings of meetings and open discussions with students prepared by teachers to conclude the level of imagination and understanding of students of different manipulations proposed by the program of the module of crystallography.

3.1. Analysis and specification

The aim is to develop an educational computer application aimed at creating three-dimensional representations of different crystalline structures. In this application we want to visualize and study these structures, and they are defined in their three dimensions and 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 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 (Baron Georges-Louis Et Bruillard Éric, 1996).

The design and development of the application developed in this work will follow three major phases, according to Table 2:

3.2. 3D modelling

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 set of tools that can model the shapes of structures in a three-dimensional way used in the application are:

| Table 2. 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 practical work 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 practical work and performs the manipulations under a teacher’s supervision. |
3.2.1. Opengl (open graphics library)

It is a very complete graphical library that is available on many platforms 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 (OpenGL Programming Guide, 2005; OpenGL Reference Manual, 2004).

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.

3.2.2. Matrices of euler

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 rotations around the x, y and z axes (respectively) used in our application are:

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

(1)

\[
R_y(\theta) = \begin{pmatrix}
\cos \theta & 0 & \sin \theta \\
0 & 1 & 0 \\
-\sin \theta & 0 & \cos \theta
\end{pmatrix}
\]  

(2)

\[
R_z(\theta) = \begin{pmatrix}
\cos \theta & -\sin \theta & 0 \\
\sin \theta & \cos \theta & 0 \\
0 & 0 & 1
\end{pmatrix}
\]  

(3)

The Figure 2 and the Figure 3 illustrate an interface that presents the first page of access to the different practical work, and a second interface presenting an example of centered cubic structure and the crystalline parameters as well as the access to the manipulation:

The verification of our models is intended to test and ensure that the modelling have been correctly developed and thus aims at the same time the capabilities of the application (Brennan & Resnick, 2012).
We have adopted another development tool to better forecast, manage and optimize our computer system. WPF (Windows Presentation Foundation) is a better graphical tool to adopt. This is a huge graphic brick of the .Net framework that can replace Windows Forms. WPF is entirely vectorial for drawing and its independent of the screen resolution, which can lead us to look for a development perspective of a mobile application offering broad access to the modeling system.

4. Evaluation and experience

The experience part of our solution is interesting to evaluate the success rate of the educational integration of our modeling application. In the university training program of the Ben M’sik Faculty of Sciences of the Hassan II Mohammedia-Casablanca-Morocco University, the crystallography module is included in the semester four of the second year of the cycle of the license for the sector “Chemical sciences”.

However, during the practical work sessions of this module, the students of the fourth semester performed the manipulations of the three manipulations of crystallography in the laboratory of physical chemistry of materials within the department of chemistry to deduce the perceptions of the teachers and students from their uses of this new computer method.
The students have already studied in the first-year computer science courses, and have used simulator software in physics and mathematics (Matlab for example). Thus, the computer science rooms of the chemistry department are equipped with all devices and tools for the installation, configuration and use of our proposed software.

The students have been fully trained in the use of the proposed application, it is prepared by the authors and under the supervision of the head of the chemistry department. However, the objective of producing documentation of the software specifications is to have a reference document for both students and teachers (registration on the platform, use of graphic interfaces, the start of manipulation, use of resources, ...). The full functionality of all specifications is realized and provided to students at the time of training.

4.1. Practical work experience 1
- 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.

4.2. Practical work experience 2
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.

4.3. Practical work experience 3
- 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.

5. Results and discussion
The objective of sampling in our case is to obtain a representative view of some students enrolled in the semester four section in the second year of chemical sciences. Because of practical reasons (time, availability of equipment, ...), it seems difficult to interview the entire population of the section.

Among different sampling methods, a random sample was used in our study because, with this method, each individual (student) in the population (section) has the same probability of being in the sample.

The total number of students enrolled in chemical sciences, who will study the crystallography module is 410. The margin of error used was 5%, it is the positive or negative deviation that we allow on the result of a survey, or the desired precision. The level of confidence reflects the degree of certainty of the margin of error and thus shows us how many times the true percentage of the population who would choose an answer is within the margin of error. In our study the margin of error is calculated for a 95% confidence level, hence a sample size of 200 students.

The selected students began 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 practical work, 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.

The teachers responsible for the practical work of the crystallography module proposed diagnostic tests that are scored out of 20 to evaluate the success rate of our computer application, as well as student engagement. The tests are represented in both groups, containing questions about the content of each manipulation, visualization, design, identification, and calculation of parameters. We have proposed a second questionnaire for students to include questions of satisfaction on improving the understanding of the practical manipulations of crystallography and communication with the new virtual environment represented by our software solution within the laboratory.

The selected students attended the computer room in the chemistry department to perform all the manipulations explained previously, according to the two modalities (traditional method and computer method). The first group of 100 students was able to visualize, identify, collect and study to conclude different properties of crystalline structures on computers thanks to our modeling application to understand crystallographic laws. The same steps of each manipulation were carried out by the second group who was able to carry out the practical work in a traditional way using the wooden models proposed in the laboratory. All the questions proposed for each manipulation are presented in the test that we have prepared to diagnose students’ comprehension (symmetry elements, coordinates, density, sites, ...).

The diagnostic tests are presented in papers to the students at the end of each practical work session, to make them in a time interval of 20 minutes for each manipulation.

The tests were supervised, and the data were collected by the teachers, to correct student responses to note and review proposals for each manipulation. We received 200 out of 20 notes to process and classify the results of our diagnostic assessment.

According to the statistics of the diagnostic tests collected for each practical work, 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 practical work:

We scheduled a practical work 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.

We found that 90.22% scored above 15/20, which represents almost 91 students out of 100 students, which seems effective for students who have tried to interact with practical work to
understand the phenomena of crystallography by a virtual simulation on a computer. Table 3 presents the percentages of students who scored above the threshold (15/20).

The following chart (Figure 4) shows the percentages of students in the first group before and after using our computer application:

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).

Evaluating the use of our simulation tool is an integral part of the teaching and learning process. Evaluating students' satisfaction consists of judging their feelings about the use of the application in order to express their opinion on the progress of crystallography tutorials. The type of evaluation practiced is “hot”, for its ease of implementation by questionnaire at the end of the training sessions.

The assessment of student satisfaction allows to:

- improve training;
- report to the sponsor on the results of the application;
- measure its efficiency;
- qualify the student benefit.

We used the Likert scale which is a psychometric tool to measure an attitude in individuals.

The satisfaction scale used for students contains four items including four answer choices that qualify the degree of agreement, as shown in Figure 5, according to two modalities of agreement (rather agree and agree) or disagree (disagreement and rather disagree). So, to measure the pedagogical efficiency of our computer application we have conducted a survey for teachers based on three levels of judgment (no high, high, very high) as shown in Figure 6.

The results have been favorable and go to achieve the educational objectives recommended for an effective integration of this computer system.

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.

| Table 3. Percentages of students who scored above 15/20 |
|-----------------------------------------------|
| Group 1 | Practical work 1 | Practical work 2 | Practical work 3 | Total result |
| Group 1 | 33.41% | 56% | 61.40% | 50.27% |
| Group 2 | 79.99% | 89.86% | 97.76% | 89.20% |
There are more simulations and computer models of the labs to study the concepts or chemical phenomena to the nanoscopic scale to facilitate their understanding and their explanation (Daaif et al., 2019).

6. Conclusion
With regard to the innovation of simulator software and educational applications, the use of digital resources in chemistry teaching is an essential part of this, which is why we have set up a computer application for the simulation of the practical work of crystallography in the laboratory.
of physical chemistry of materials of the Faculty of Sciences Ben M’sik. The adaptation of a virtual laboratory presented using a three-dimensional graphics platform allows students to study different crystalline structures and identify different parameters and crystallographic characteristics. The objective of this work is to optimize and renovate teaching practices according to the didactical factors of chemical science, the scientific and experimental factors explained above.

The results were benevolent, and 89.20% of students in the first group of 100 people who used the simulation scored above 15/20, and 90.22% of the second group (100 students) obtained a maximum score (greater than 15/20) according to the two methods (traditional and computer). Teachers indicated that the motivation to continue the integration of information and communication technologies will lead us to study other practical work for better integration of simulation and modeling applications.
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