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Virtual and Augmented Reality Environments to Learn the Fundamentals of Crystallography

Jamil Extremera [1], Diego Vergara [2,*], Lilian P. Dávila [3] and Manuel P. Rubio [4]

[1] Computer Science and Automatics, University of Salamanca, 37008 Salamanca, Spain; jamil.extremera@usal.es
[2] Technological Department, Catholic University of Ávila, 05005 Avila, Spain
[3] Department of Materials Science and Engineering, School of Engineering, University of California at Merced, Merced, CA 95343, USA; ldavila@ucmerced.edu
[4] Construction Department, University of Salamanca, 49029 Zamora, Spain; mprc@usal.es
* Correspondence: diego.vergara@ucavila.es; Tel.: +34-920-251-020

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Abstract: Nowadays, there are many situations in which information and communications technology (ICT) is used as a vehicle to transmit knowledge. The fast evolution of technology in recent decades has favored the development of virtual reality (VR) and augmented reality (AR) and with them the emergence of virtual laboratories (VLs) using VR or AR. Since such technologies can help students understand the atomic spatial distribution, crystallography is a discipline that has taken advantage of the use of VL in the teaching of crystal lattices, thus solving the usual educational problem of visualization in two- and three-dimensions. This paper presents a literature review that helps to identify the main features of VLs (based on VR or AR) that have been developed in the academic field to support the learning of crystallography concepts. Furthermore, this paper describes a VL developed by the authors where students can learn the main contents related to the 14 Bravais lattices (unit cells, directions, crystallographic planes, interstitial sites, etc.) by exploring the stands of a virtual museum. Such a VL uses non-immersive VR and has been designed based on the authors' long-term research to achieve a high learning effectiveness educative platform.

Keywords: crystallography; crystalline structures; Bravais lattices; materials science and engineering; virtual reality; augmented reality; virtual reality learning environments; virtual laboratory; spatial comprehension

1. Introduction

The teaching and learning process of crystal lattices is characterized by presenting difficulties of spatial visualization when having to mentally recreate complex spatial distributions [1]. Both the spatial distribution of the atoms that make up the unit cells and the structures that are formed by joining them can be concepts that are difficult for many students to understand when using teaching methods based solely on two-dimensional graphic representations (as, for example, in the drawings of traditional textbooks). To address this problem, typically, models made of polymeric materials or wood have been used to replicate the shape of crystallographic structures [2]. However, this practice has disadvantages such as high cost of commissioning the manufacture of new custom-made models [2] or the limitations of its handling (e.g., it is difficult to create sections of the unit cells to visualize planar density or linear). On the other hand, in the last decades, tools based on information and communications technology (ICT) have been developed that aim to improve the spatial understanding that students have when they approach the learning of crystallographic structures.

In this sense, crystallographic structure repositories are known, such as those that are stored in databases such as the Crystallography Open Database (COD) [3] or the one that is hosted in the Cambridge Crystallographic Data Center (CCDC) [4]. This data can be downloaded for later processing in programs such as VESTA [5] or Mercury [6,7], which offer a multitude of crystallographic analysis options, among which are different choices for viewing and exploring three-dimensional crystallographic models of crystallographic networks.

Another example of the use of ICT applied to the teaching of crystallography is found in 3D printing. Thanks to the reduction and expansion that 3D printers have experienced, there are several works [2,8–10] that describe methods to create three-dimensional impressions of customized crystallographic structures. These physical models are subsequently freely explored by the students in the same way that would be done with traditional models made of polymeric materials or wood, but offer a series of advantages with respect to the former, such as: (i) the creation of rapid and low-cost physical models given the low price that 3D printers currently have and the material used in printing, (ii) the possibility of printing structures hosted in COD or CCDC [8], (iii) the possibility of customizing the size of the elements that make up the crystallographic structures [8], and (iv) the possibility of printing complex structures [2], among others.

Conversely, the rapid evolution that ICT has undergone has favored that in recent years there has been a great development of virtual reality (VR) and augmented reality (AR) technology [11,12]. Indeed, although VR was conceptually defined in 1965 by Ivan Sutherland [13] as the way to make the virtual world shown on the screen look, sound, and feel real, it was not until well into the last decade that hardware has allowed the improvement and cheaper and consequent expansion of VR and AR in the educational sectors. These technologies allow the creation of didactic tools with high efficiency at the formative level, improving the teaching-learning process in university training [14–22]. Some of the cases in which the use of this technology is especially useful are in those where it is required to improve students' spatial understanding to help them comprehend concepts related to complex spatial structures [1,23–27], as is the case with learning crystallographic structures.

There are currently various computer applications that use VR (both immersive and non-immersive) and AR to support the teaching of different aspects related to crystallography. By way of clarification, immersive VR (IVR) is one that immerses the user in the virtual environment, normally through a VR glasses system known as a head-mounted display (HMD), while non-immersive VR (NIVR) is one that usually shows the virtual environment on flat screens of standard devices such as computers or smartphones [28,29]. To know the state of the art, that is, what ICT tools based on VR and AR have been created in the academic field so far to support the teaching of crystallography, the authors of this article have carried out a systematic search in two multidisciplinary databases: (i) Web of Science (WOS) and (ii) Scopus. This article presents the exact methodology that has been followed to perform the systematic search, in addition to describing each of the relevant results that this search has yielded.

Virtual reality learning environments (VRLEs) are applications that are based on the use of VR to create virtual learning environments and both their development and use in university classrooms have been studied in different works [15,19–22,30–33]. Different works by Vergara et al. [29,34–37] describe the process that must be followed to create and use a VRLE, addressing the process that includes the initial considerations, design, development, use in the classroom, evaluation, and improvement. The methodology described in these studies allows the creation of VRLEs that facilitate students to achieve a high level of meaningful learning (i.e., that the knowledge taught is fully understood by the student and is able to relate it to other previously learned concepts [34]), in addition to ensuring that the effectiveness at the formative level of these tools does not decrease over the years due to technological obsolescence [35]. Based on what is described in these studies, the authors have developed a VRLE that aims to serve as a tool for engineering students who approach learning the 14 Bravais networks. This article describes the design and development parameters that have been incorporated into this VRLE, which allow to infer that it will be an effective tool in teaching basic concepts of crystallography.

2. Systematic Literature Review

The systematic search carried out by the authors seeks to know what tools based on VR and AR have been developed so far in the academic field to support the teaching of concepts related to crystallography. For this, two search equations have been designed, one to be run on the WOS platform and the other for the Scopus database. The fact that a different search equation has been created for each system is because each one uses different terminology and search terms (e.g., in WOS the expression "crystal" returns results that contain the exact term "crystal", while in Scopus this same expression returns both the term "crystal" and its plural form "crystals").

The search equations have been designed to index those works related to the teaching of crystallography and that make use of VR or AR. For this, the search for terms has been carried out in the fields of title, abstract and keywords, in such way that the following terms are contained in one or more of the mentioned fields: (i) "crystal" (or any of its variants, such as crystallography, microcrystalline, etc.) or "nanostructure" (or its plural, "nanostructures"), (ii) terms related to teaching (all variants of teaching, learning, training or education), and (iii) terms related to VR or AR technology (the exact expressions virtual reality, augmented reality, the variants of virtual laboratory, the singular/plural of virtual environment or the concept of didactic virtual tool). Table 1 lists the expressions used in the search equations and examples of terms that databases return.

Table 1. Expressions used in the search string and examples of words returned by databases.

Expression Used in the Search String	Examples of Words Returned by Databases
crystal	crystallography, crystalline, microcrystalline
nanostructure$ [1]	nanostructure, nanostructures
teach*	tech, teaching
learn*	learn, learning
train*	train, training
educati*	education, educative
"virtual reality"	virtual reality
"augmented reality"	augmented reality
"virtual lab*"	virtual lab, virtual labs, virtual laboratory
"virtual environment$" [1]	virtual environment, virtual environments
"didactic virtual tool$" [1]	didactic virtual tool, didactic virtual tools

[1] $ symbol to be used in WOS only.

The literature search has not been temporarily bounded in either WOS or Scopus and, therefore, publications have been indexed from the present to the oldest included in each database. Each search process has been refined to allow for the indexing of all types of publication (articles, proceedings, book chapters, etc.) and to exclude those papers that are written in a language other than English. The date of the searches described in the following sections (both in WOS and Scopus) is 1 May 2020.

2.1. Search Results in WOS

The search on the WOS platform has been carried out in its core collection database, including all its indexes. Since the advanced search in WOS allows to search simultaneously in the title, abstract and keywords using only the field "topic" – which is identified with the field tag TS-, the search criteria used was the following:

TS = ((*crystal* OR nanostructure$) AND (teach* OR learn* OR train* OR educati*) AND ("virtual reality" OR "augmented reality" OR "virtual lab*" OR "virtual environment$" OR "didactic virtual tool$"))

The results obtained using this search equation have been refined as previously described (i.e., without temporal dimensioning, allowing to index all types of publications and excluding those that are not written in English). In this way, 43 search results have been obtained, the oldest of which was from 1997 [38].

2.2. Search Results in Scopus

Scopus itself constitutes a single database and, therefore, it is not necessary to select a specific database in which to perform the search, which has been carried out using the fields "title", "abstract" and "author keywords". Thus, the search criteria used were as follows:

TITLE((*crystal* OR nanostructure) AND (teach* OR learn* OR train* OR educati*) AND ("virtual reality" OR "augmented reality" OR "virtual lab*" OR "virtual environment" OR "didactic virtual tool")) OR ABS((*crystal* OR nanostructure) AND (teach* OR learn* OR train* OR educati*) AND ("virtual reality" OR "augmented reality" OR "virtual lab*" OR "virtual environment" OR "didactic virtual tool")) OR AUTHKEY((*crystal* OR nanostructure) AND (teach* OR learn* OR train* OR educati*) AND ("virtual reality" OR "augmented reality" OR "virtual lab*" OR "virtual environment" OR "didactic virtual tool"))

As in the case of WOS, the results obtained using this search equation have been refined as previously described (i.e., without temporal dimensioning, allowing to index all types of publications and excluding those that are not written in English). In this case, 59 results have been obtained, of which the oldest paper was published in 1995 [39].

2.3. Analysis of Indexed Results (WOS and Scopus)

As noted in the previous sections, WOS has returned 43 results and Scopus 59, with 23 of them being duplicate results (they are indexed in both the WOS and Scopus searches). After eliminating the duplicate results, the total number of unique results indexed between the two systems is 79. Of these 79 unique results, after analyzing the content of the abstract of each one, only those works that describe platforms based on VR or AR and that are focused on understanding concepts related to crystallographic structures are selected. Thus, a total of 13 relevant works has been identified, all of them in a paper, proceeding or book chapter format. The process followed to carry out the search and select the relevant works is summarized in the schematic shown in Figure 1.

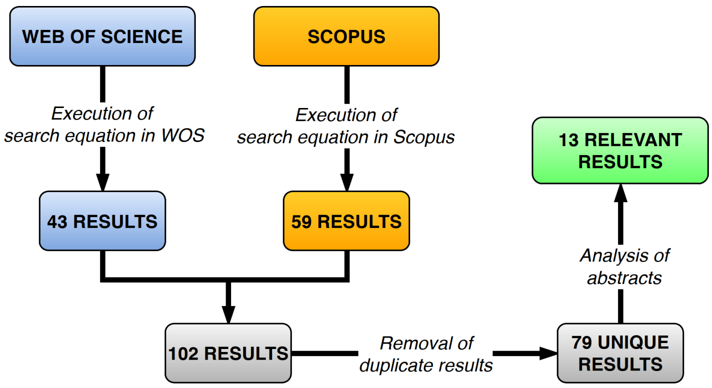

Figure 1. Summary of the literature review process followed to select the relevant research works in the instruction of fundamentals of crystallography by virtual learning environments.

The titles of the 13 selected works are listed below, along with the year of their publication:

- Recent developments in virtual reality-based education, 1996 [40].
- Collaborative augmented reality for inorganic chemistry education, 2008 [41].
- Learning about the unit cell and crystal lattice with computerized simulations and games: A pilot study, 2010 [42].
- New augmented reality applications: Inorganic chemistry education, 2011 [43].
- Development of an educational virtual transmission electron microscope laboratory, 2014 [44].
- An immersive 3D virtual learning environment for analyzing the atomic structure of MEMS-relevant materials, 2015 [45].

- Beyond the flipped classroom: A highly interactive cloud-classroom (HIC) embedded into basic materials science courses, 2016 [46].
- A virtual resource for enhancing the spatial comprehension of crystal lattices, 2018 [47].
- Can virtual reality enhance learning: A case study in materials science, 2018 [48].
- NOMAD VR: Multiplatform virtual reality viewer for chemistry simulations, 2018 [49].
- A virtual laboratory for learning fullerene production and nanostructure analysis, 2018 [50].
- Application of virtual reality for learning the material properties of shape memory alloys, 2019 [51].
- Visualizing 3D molecular structures using an augmented reality app, 2020 [52].

The virtual platforms described in each of the previous works are described individually in the following section, except for [41] (published in 2008) and [43] (published in 2011), since both have been written by the same author, have been developed at the same university and describe the same type of platform. In particular, the work described in [43] can be interpreted as a more detailed extension of the work described in [41], and for this reason, only the platform exposed in [43] is described.

Figure 2 shows thumbnails of images extracted from each work [40–52] to offer the reader a clearer idea of the look of the platforms described. In addition, Figure 2 classifies the described platforms according to the technology used by each of them: NIVR [40,42,44,47], IVR [45,48,49], IVR and NIVR [50,51], and AR [41,43,46,52].

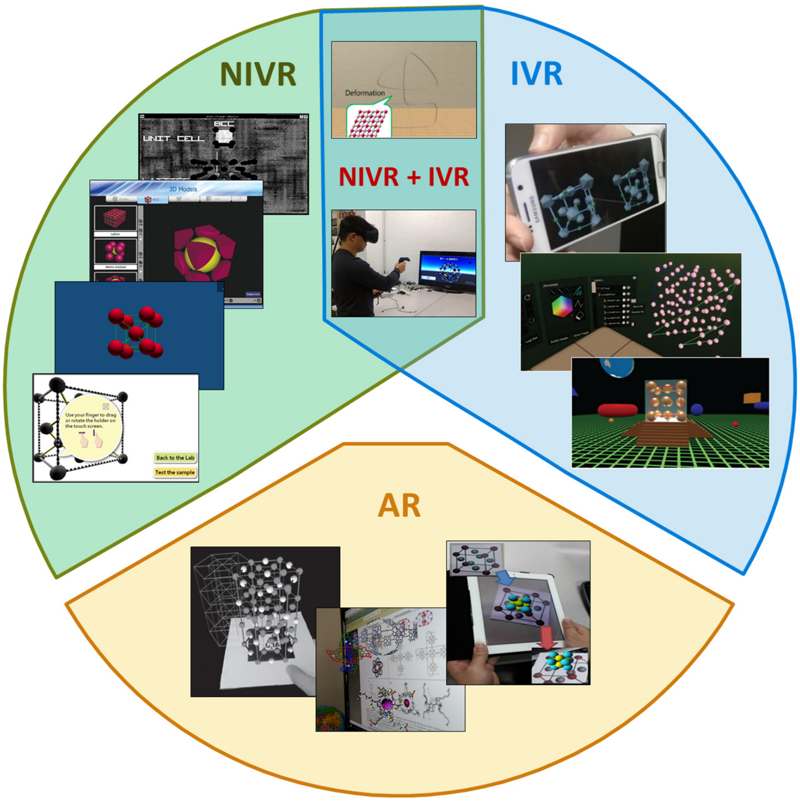

Figure 2. Thumbnails of the described platforms and their classification according to the used technology (NIVR, IVR or AR).

3. Description of the Relevant Works

This section presents a summary description of the virtual crystallographic network platforms presented in each of the thirteen research works [40–52] selected through the systematic search. Each description has been made in such a way that it includes the following data (as long as they are available in their corresponding work): (i) year of the first publication of the work in which the platform is presented; (ii) concepts it aims to teach and its relation to crystallography; (iii) type of technology used, that is, NIVR, IVR, or AR; (iv) hardware used to use the application; (v) description and object of the study carried out on the task; and (vi) other data. Table 2 summarizes these aspects for each of the research works considered. Note that, in Table 2, the column labeled "year" refers to the year of the first publication of the work. For sake of clarity, the following terminology has been used from now on: BCC (body-centered cubic), FCC (face-centered cubic), HCP (hexagonal close-packed), DC (diamond cubic), TEM (transmission electron microscope), MEMS (micro-electro-mechanical systems), SMA (shape memory alloy), PC (personal computer), and CAVE (cave automatic virtual environment).

Table 2. Summary of the main features of each platform studied.

Article	Year	Main Crystallographic Concepts Taught	Technology	Hardware	Study Included
[40]	1996	• BCC cells • Lattices	NIVR	• PC	No
[42]	2010	• Primitive cubic cells • BCC cells • FCC cells • HCP cells • Lattices	NIVR	• PC	Yes
[43]	2011	• BCC cells • FCC cells • HCP cells • Tetrahedral structures • Bravais lattices • Crystallographic planes	AR	• PC • Markers	Yes
[44]	2014	• Use of TEM • Crystal structure and diffraction patterns of diamond, graphite and TiO_2	NIVR	• Smartphone • Tablet	Yes
[45]	2015	• Atomic structure of monocrystalline materials relevant to MEMS	IVR	• PC & HMD • Controller	No
[46]	2016	• Primitive cubic cells • BCC cells • FCC cells • HCP cells	AR	• Smartphone • Tablet • Markers	Yes
[47]	2018	• Primitive cubic cells • BCC cells • FCC cells • Bravais lattices	NIVR	• PC	Yes
[48]	2018	• BCC cells • FCC cells • DC cells • HCP cells	IVR	• PC & HMD • Controller	Yes
[49]	2018	• Any type of unit cell • Lattices • Complex structures • Evolution of chemical reactions	IVR	• PC & HMD • CAVE • Smartphone • Controller	Yes
[50]	2018	• Use of TEM • Structure and diffraction patterns of fullerenes	IVR / NIVR	• PC & HMD • Controller • Smartphone • Tablet	Yes
[51]	2019	• SMA atomic structure modification	IVR / NIVR	• PC & HMD • Controller • Smartphone • Tablet	Yes
[52]	2020	• Any type of atomic structure	AR	• Smartphone • Tablet	No

3.1. Reference [40]: Recent Developments in Virtual Reality Based Education

This work was published in 1996 and it presents an application divided into modules, each module is dedicated to teaching a concept related to chemistry. In one of these modules, the arrangement of the atoms in a unit cell of the BCC type is taught, as well as the crystalline structure that forms the union of several unit cells of this type. The type of technology used by this application is NIVR and runs on a PC. As indicated in the work, at the time of publication this module had not yet been evaluated with students and therefore does not include the corresponding analysis.

3.2. Reference [42]: Learning about the Unit Cell and Crystal Lattice with Computerized Simulations and Games: A Pilot Study

This work was published for the first time in 2010 and it presents two modules oriented to the teaching of cubic primitive unit cells (BCC, FCC, and HCP) as well as the crystalline structure that forms the union of several unit cells of these structure types. The type of technology used by this application is NIVR and runs on a PC. This investigation includes a study in which 23 science students used the application and answered questionnaires whose responses were subsequently analyzed by the authors of the work. The purpose of this study was to determine the effectiveness of the application by improving the learning of the unit cells and crystallographic networks, in addition to evaluating the opinion of students after using the application.

This application is divided into two main modules. The first module allows: (i) freely exploring the unit cells and the networks they form; (ii) learn a method to deduce the unit cell from a crystal lattice; (iii) visualize how a crystal lattice is generated by moving the unit cell along the three main orthogonal planes. The second module of the application consists of a game in which the user must collect atomic pieces that belong to a unit cell to later place these pieces in the place of the corresponding unit cell. This type of platform with two modules, one that develops the theoretical part using VR and the other with educational exercises, is quite common [14,53].

3.3. Reference [43]: New Augmented Reality Applications: Inorganic Chemistry Education

This work was first published in 2011 and constitutes a continuation of the platform presented in a previous work of the same authors in 2008 [41]. The objective of this platform is to teach concepts related to unit cell of type BCC, FCC, HCP as well as Bravais lattices, tetrahedral structures, crystallographic planes or sets of unit cells. The type of technology used by this application is AR, running on a PC to which several cameras are connected to capture images of the real environment and detect certain markers. Each of these markers has a certain virtual element associated (e.g., a certain unit cell). The images captured by the cameras are superimposed with the virtual elements associated with each marker and displayed on a screen by using a projector. This platform allows the user to move and rotate the markers to change the point of view of the virtual elements displayed through the projector. The objective of this study was to find out the opinion of the students about the educational platform. In this investigation, 15 students from the University Jaume I (Spain) participated in course subjects ranging from Materials Sciences, Ceramic Inorganic Chemistry, and Advanced Chemistry Laboratory. After using the application, the students filled out surveys whose results were later analyzed by the authors of the work. The conclusions of the study indicate a high acceptance of this platform by the students.

3.4. Reference [44]: Development of an Educational Virtual Transmission Electron Microscope Laboratory

This work was published for the first time in 2014 and it presents a platform that aims to teach how to use a TEM, on the one hand, and the crystal structure of three materials and their respective diffraction patterns, on the other hand. The type of technology used by this application is NIVR and runs on a smartphone or tablet, carrying out the interaction between the user and the application through the touch screen of the given device. This study aimed to evaluate the effectiveness of the application in teaching nanostructural analysis. Thirty-eight students from the Department of Applied Science at the University of Hsinchu (Taiwan) and 36 other students (mostly high school students) participated in the study, who used the application or viewed instructional videos, before and after which they filled in questionnaires whose answers were later analyzed by the authors of the work. The study concluded the learning achievement of the students who used the platform was superior to that obtained by the students who viewed videos. Also, the students who used the platform rated it positively.

This application recreates a virtual TEM that the user can learn to operate using information that the application itself offers. The crystalline structures of three materials (diamond, graphite, and titanium oxide) are presented, which the user can rotate to become familiar with the spatial arrangement of the atoms that make up their structures. After exploring the crystalline structures, the user can carry out the observation in the microscope of each one of the material samples and observe the diffraction pattern obtained for each one of them. Finally, the user can perform an online test to assess the level of knowledge acquired.

3.5. Reference [45]: An immersive 3D Virtual Learning Environment for Analyzing the Atomic Structure of MEMS-Relevant Materials

This work was published in 2015 and it presents a platform that aims to teach concepts related to the atomic structure of monocrystalline materials used in MEMS (e.g., silicon, chromium, titanium, and copper). The type of technology used by this application is IVR, visualizing the virtual environment using an HMD connected to a PC and carrying out the interaction between the user and the virtual environment using a game controller. This study did not include any statistical study with students.

This application allows access to a laboratory in which the user can select and read relevant information about a material. Subsequently, the user can interact in real-time with the atomic structure of the previously selected material, analyzing key parameters of the crystal lattice such as the number of atoms in the lattice, atomic packing factor, linear atomic density, etc.

3.6. Reference [46]: Beyond the Flipped Classroom: A Highly Interactive Cloud-Classroom (HIC) Embedded into Basic Materials Science Courses

This work was published for the first time in 2016 and it presents a platform that aims to teach materials science concepts. This platform contains two modules, one of them focused on the teaching of the cubic primitive type unit cells (BCC, FCC and HCP). The type of technology used by this application is AR and runs on a smartphone or tablet, carrying out the interaction between the user and the application through the touch screen of these devices, requiring the use of the integrated photo camera on the device.

This work evaluates the educational effectiveness of using the AR platform in a Materials Science course, comparing it with traditional teaching methodology. In this study, 92 second-year students from the University of Science and Technology (Taoyuan County, Taiwan) participated. They were divided into two groups that received the same materials science course but in two different modalities: through the platform (experimental group) and following the traditional teaching methodology (control group). Both before and after receiving the course in either of the two modalities, the students answered questionnaires whose answers were later evaluated by the authors of this work. The study concluded that students who used the AR platform had better results across three analyzed learning dimensions (knowledge, comprehension and application in a basic materials course) compared to those students who had not used it.

This application allows the user to focus on the camera of a smart device (smartphone or tablet) on a certain image of a unit cell (instead of a market such as those commonly used in AR-based applications) so that an image appears on its 3D cell unit under study. The user can then, by using the touchscreen, rotate the unit cell to see it from different angles, view interactive animations and videos, etc.

3.7. Reference [47]: A Virtual Resource for Enhancing the Spatial Comprehension of Crystal Lattices

This work was first published in 2018 and it presents a platform that aims to make it easier for students to understand the position of atoms within crystal lattices. The type of technology used by this application is NIVR and runs on a PC. This study aimed to know the opinion that students have about various aspects of the platform. Forty Mechanical Engineering Degree students at the Catholic University of Ávila (Ávila, Spain) received master's level courses on Bravais networks, used the platform, and solved exercises, after which each student answered questions via a survey. The study concluded that students rated positive aspects of the use, design, and teaching effectiveness of the platform.

This application allows the user to choose one of the 14 Bravais networks (which are grouped into seven crystalline systems) to carry out on each one them different operations such as rotating and obtaining views of sections or their expanded set.

3.8. Reference [48]: Can Virtual Reality Enhance Learning: A Case Study in Materials Science

This work was first published in 2018 and it describes a method of using the Arthea Visualizer [54] to teach concepts related to BCC, FCC, DC, and HCP type of unit cells. The type of technology used by this application is IVR, visualizing the virtual environment using an HMD connected to a PC and carrying out the interaction between the user and the virtual environment using a controller. The objective of this study was to evaluate the usability and effectiveness of the teaching method described in it (based on the use of Arthea). Students from STEM (science, technology, engineering, and mathematics), six of them undergraduate and one graduate, at the University of Michigan (USA) participated in this study. During the investigation, a group of students carried out a series of activities using Arthea while another group of students carried out the same activities using paper and pen. After completing the activities, the students answered a questionnaire whose results were analyzed by the authors. Although the number of participating students in this study was very small, the authors noted that issues related to spatial reasoning were best resolved by those who had used Arthea.

The teaching method revealed in this work consists of creating 3D models of unit cells and crystalline networks to later visualize them on an HMD using the Arthea application. Arthea allows visualizing 3D models in different HMD systems, as well as making drawings on them [48,54].

3.9. Reference [49]: NOMAD VR: Multiplatform Virtual Reality Viewer for Chemistry Simulations

This work was published for the first time in 2018 and it presents a platform that aims to visualize both atomic structures and chemical reactions at the atomic level. The type of technology used by this application is IVR, allowing the virtual environment to be viewed using different types of hardware: HMD connected to a PC, HMD with a smartphone attached in front of the user's eyes, and CAVE system. To facilitate the reader's understanding, the CAVE system projects images on all the surrounding walls, ceiling, and floor of a room so that users, equipped with stereoscopic goggles, are immersed in a three-dimensional virtual environment [28,55]. The interaction between the user and the application is generally carried out through a controller. This study does not include any statistical study with users of the platform.

The platform described in this work is not only intended to serve as an educational tool but also has other objectives, such as serving as a tool for researchers. This platform constitutes a visualizer that can be used to visualize the result of common computer simulations of the evolution of chemical reactions and other interesting data representations used in materials science, such as unit cells and crystallographic networks. This platform allows viewing in three dimensions materials science datasets created by the user as well as datasets obtained from the repository for materials science data NOMAD [56].

3.10. Reference [50]: A Virtual Laboratory for Learning Fullerene Production and Nanostructure Analysis

This work was published for the first time in 2018 and it presents a platform that aims to teach concepts related to the fullerenes as well as familiarizing students with how a TEM works. This application can use two types of technology: (i) IVR, visualizing the virtual environment through an HMD connected to a PC, carrying out the interaction between the user and the virtual environment through a controller, and (ii) NIVR, displaying the virtual environment on a smartphone or tablet, carrying out the interaction between the user and the application through the touch screen of the device being used. This study aimed to evaluate the effectiveness of the application in teaching production and analysis of fullerenes, for which sixty-seven students from a senior high school at Hsinchu (Taiwan) participated. A control group viewed instructional videos while the experimental group used the educational platform, before and after which they filled in questionnaires whose answers were later analyzed by the authors of the work. The study concluded that the learning achievement of the students who used the platform was superior to that obtained by the students who viewed videos. Also, the students who used the platform rated it positively.

This application allows the user to produce fullerenes with an arc-discharge apparatus and use a TEM to observe their geometrical structure and diffraction pattern. Furthermore, the platform has a module that allows the user to perform the assembly of fullerene structures by moving carbon atoms to the bonding position one by one. Once the assembly of a fullerene is completed, the application allows the user to send the created model to a 3D printer to fabricate a corresponding physical model.

3.11. Reference [51]: Application of Virtual Reality for Learning the Material Properties of Shape Memory Alloys

This work was published for the first time in 2019 and it presents a platform that aims to teach concepts related to SMAs. Among the concepts taught is the variation that the crystalline structure undergoes when passing from the martensite phase to the austenite phase and vice versa when the material is subjected to successive deformation-heating-cooling processes. This application can use two types of technology: (i) IVR, visualizing the virtual environment through an HMD connected to a PC, carrying out the interaction between the user and the virtual environment through a controller, and (ii) NIVR, displaying the virtual environment on a smartphone or tablet, carrying out the interaction between the user and the application through the touch screen of the device being used. The purpose of this study was to measure the performance of this platform in learning the SMAs properties and applications. A total of 132 students from the Department of Materials Science at a university in North Taiwan participated in this study. The students were divided between a control group, which carried out a real experiment, and an experimental group, which performed the same experiment but virtually using the educational platform. Both before and after the experiment (real or virtual), the students filled out questionnaires whose results were subsequently analyzed by the authors of this work. The study concluded that the learning effectiveness of the platform was higher than performing the real experiment. Moreover, the students reported positive feedback to the use of the platform.

This platform allows the user to interactively learn concepts related to SMAs, such as their crystalline structure or practical applications. Among other options, this platform allows one to carry out virtually a process by which a wire of a SMA is successively deformed, heated, and cooled to show (in a simplified way) the different configurations that its crystalline structure adopts.

3.12. Reference [52]: Visualizing 3D Molecular Structures Using an Augmented Reality APP

This work was first published in 2020 and it presents a methodology to create an application that allows the user to visualize in 3D any molecular structure based on crystallographic data or from computer modeling. This work describes a platform developed according to this methodology and which serves to visualize complex structures (i.e., the porphyrin nanoball). The type of technology used by this application is AR and it runs on a smartphone or tablet, requiring the use of the integrated photo camera on the device. This paper does not include a study of the described platform, but it is noted that 24 students from a high school in Denmark used it successfully.

The applications created following the methodology described in this work allow the user to focus on the camera of a smart device (smartphone or tablet) on a certain image of an atomic structure (instead of a market such as those commonly used in AR-based applications). In this way, the three-dimensional atomic structure superimposed on the real environment appears on the smart device's screen, making it possible to move the device to view it from different angles.

4. VRLE for Teaching Bravais Lattices

A VRLE developed by the authors is presented in this section. This VRLE, which serves to support the university education of the 14 Bravais networks, is presented as a NIVR-based application that runs on a PC, with the interaction between the user and the application being carried out using a keyboard and a mouse. The appearance and handling of this VRLE are similar to that of a first-person shooter video game, in which the user can freely explore the facilities of a museum (i.e., exhibition hall, office, bathroom and classroom), most of them are shown on Figure 3. When the user accesses the museum's exhibition hall, she or he finds 14 stands (Figure 3b), each of which shows one of the Bravais networks. By approaching each stand, the user can obtain specific data on the crystal lattice it contains (e.g., atomic packing factor, coordination number, or the number of atoms per unit cell) as well as to choose between different display options, whose aim is to reinforce the spatial comprehension of the crystal lattice (Figure 4): (i) full rotation and translation of the lattice; (ii) different views of the lattice (the unit cell only, the expanded lattice, etc. Figure 4b–e); (iii) tetrahedral and octahedral interstitial voids (in both the unit cell and the expanded lattice); (iv) crystallographic directions and planes, indicating the corresponding Miller indices (in both the unit cell and the expanded cell); (v) families of both crystallographic directions and planes; and (vi) gathering of specific sections or subsets of data. This VRLE was designed with a high level of interactivity, thus favoring the user a better spatial comprehension of the concept of crystal lattices. A complementary video is available in the Supplementary Material of this paper so that the reader can better visualize all the options shown in Figure 4.

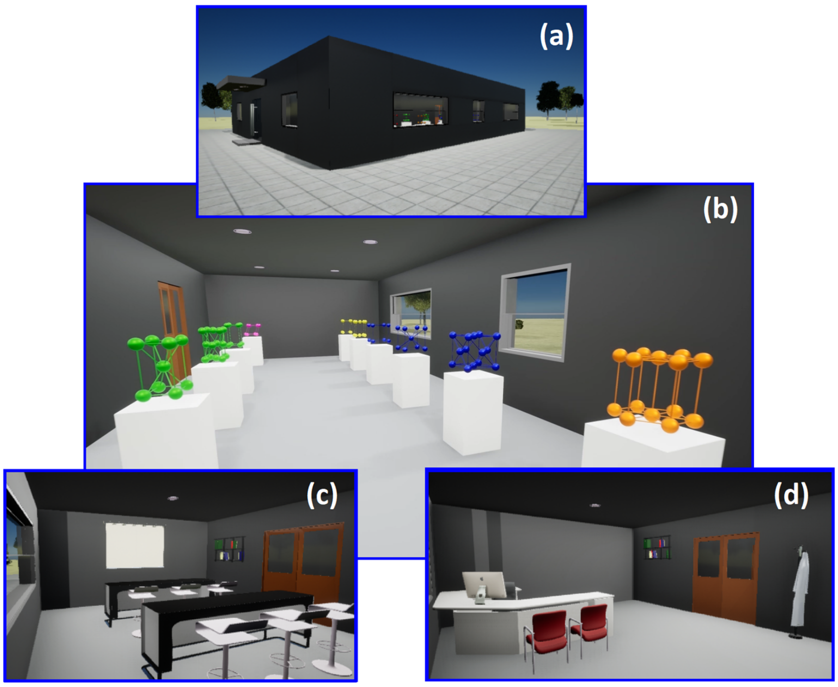

Figure 3. Screenshots of the museum facilities that users can freely explore: (**a**) exterior view of the building; (**b**) crystal lattices exhibition hall; (**c**) classroom; and (**d**) office.

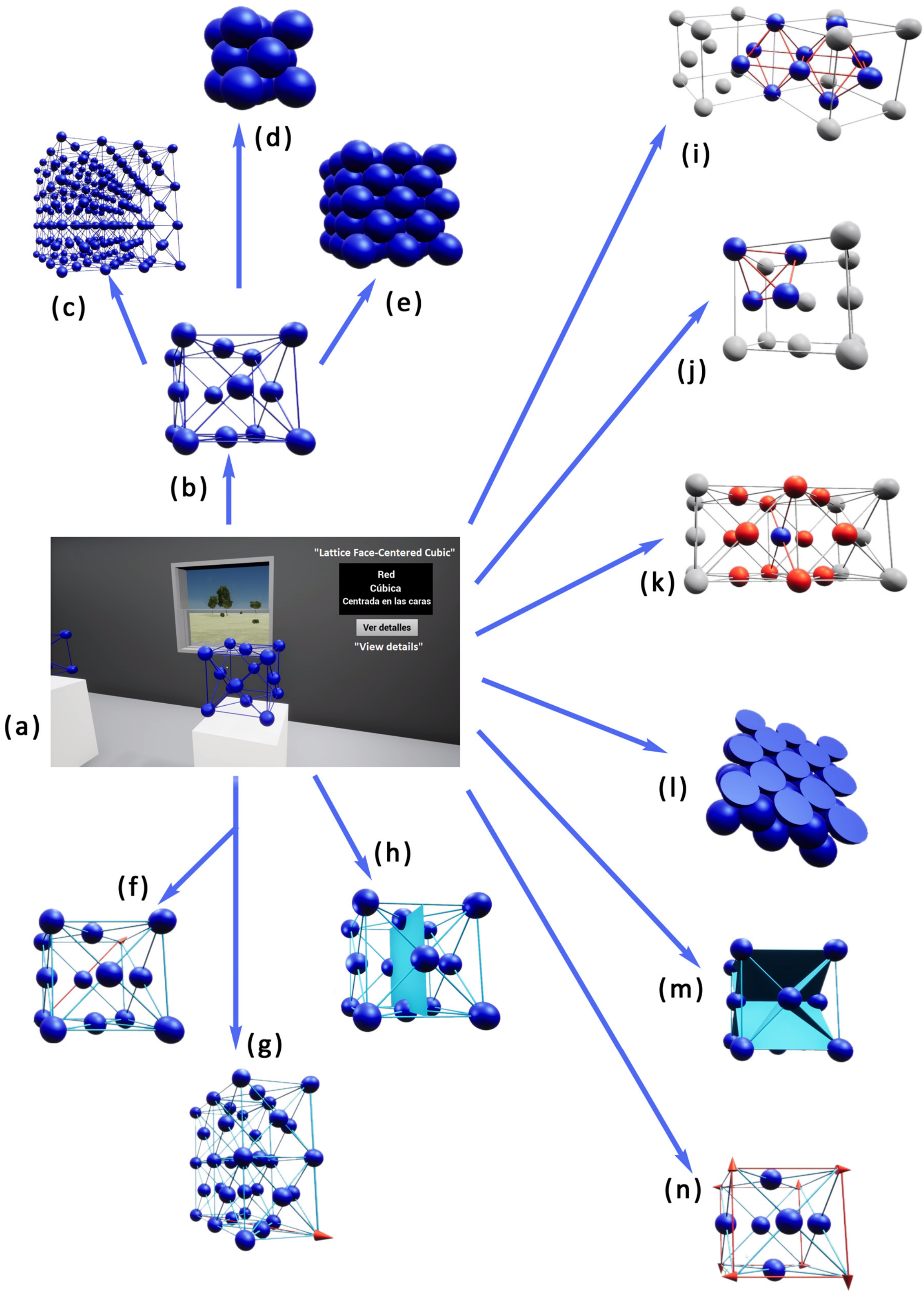

Figure 4. Different views of a material structure available in the VRLE showing: (**a**) lattice FCC; (**b**) expanded unit cell; (**c**) expanded set; (**d**) unit cell in CPK mode; (**e**) super set in CPK mode; (**f**) crystallographic direction [011]; (**g**) crystallographic direction [210]; (**h**) crystallographic plane [020]; (**i**) octahedral interstitial sites (voids); (**j**) tetrahedral interstitial site (void); (**k**) coordination index; (**l**) cross-section; (**m**) family of planes {110}; and (**n**) family of directions <100>. In part (**a**) the translation of text in Spanish to English is indicated inside the image.

This VRLE has been developed considering the results obtained from previous studies carried out by Vergara et al. [29,34–36]. These investigations detail: (i) the methodology that must be followed to create a VRLE, use it in the classroom, evaluate it, and subsequently improve it [29,34,35], and (ii) factors that must be taken into account to achieve a high degree of effectiveness at the formative level [34,36]. A flowchart is shown in Figure 5, which summarizes the steps followed to develop and implement such a VRLE in the classroom.

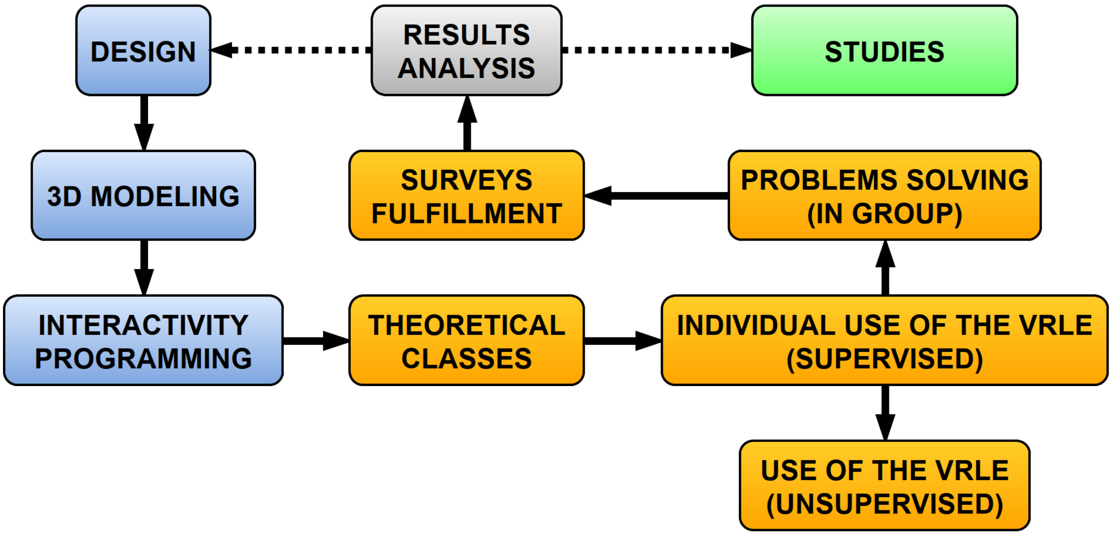

Figure 5. Summary of the methodology followed during the development of the VRLE and its implementation in the classroom.

4.1. Development

The first stage of development has consisted of defining in detail the design parameters of the VRLE, which are summarized as follows:

- what concepts it intends to teach: all those related to the teaching of Bravais networks at the university level
- what type of VR technology to use: NIVR
- what hardware will be necessary to run the application: mid-range PC
- how the user will interact with the application: keyboard and mouse
- what form of virtual environment: a museum (Figure 3)
- way in which the user will learn the concepts: approaching each stand of the museum and selecting one of the different options that are provided (cf. Supplementary video).

The next stage of development has been to three-dimensionally model the virtual environment and all its associated elements. At this stage, materials and textures have also been applied to the different virtual elements and the different stages have been illuminated. To carry out this activity, a recent version of 3DS Max® (version 2019, Autodesk, San Rafael, CA, USA, 2018) has been used. An important advantage of this program is the availability of a large amount of open access (at no cost) information on the internet about its management, as well as the solution to possible problems that may arise during its use.

The last phase of development consists of providing the virtual environment and the elements it contains with the interactivity necessary to be able to use it. In this stage, the following is programmed, among others: how the user moves around the stage, buttons that appear on the screen, actions that can be carried out on crystallographic networks or automatic movements (e.g., opening doors), etc. To carry out this programming, a recent version of the Unreal Engine 4® game engine has been used (UE4, version 4.21, Epic Games, Cary, NC, USA, 2018). UE4 uses object-oriented programming and allows the user to program a large number of functionalities using visual scripting, which avoids the need to write code, thus saving programming time (however, UE4 also allows the user to program more complex functionalities by typing C++ code). Additionally, UE4 incorporates advanced features in generating the visual appearance of virtual environments, such as physically-based rendering materials, realistic lighting effects indoors and outdoors, and latest rending techniques such as real-time ray tracing that uses calculation algorithms based on the laws of optics. This results in visually more realistic environments.

4.2. Use in the Classroom

The use of VRLE in the classroom is currently being implemented in the Materials Science and Engineering classes received by second-year Mechanical Engineering students at the Catholic University of Ávila (Spain). At first, the instructor gives master level courses (2–4 h) in which he/she explains the Bravais networks theory. At the end of these courses, students individually use the VRLE in the classroom under the supervision of the instructor for 30–60 min, and are able to continue using it unsupervised outside school hours as long as they wish. Subsequently, students formed teams of 2–4 individuals to solve an exercise for approximately two hours. Finally, the students filled out surveys from which the researchers extracted data whose analysis allows to understand, among others, the following aspects of the VRLE: (i) training effectiveness, (ii) acceptance by the students, and (iii) aspects of the program that require improvements.

5. Discussion

Through the systematic literature review carried out in this work, a total of 12 platforms of this type have been identified, which have been developed in 25 years. On the other hand, it is observed that all the platforms described (except for [51]), exploit the 3D visualization possibilities offered by VR and AR to help understand the arrangement that atoms and molecules have in space. It is also observed that, in most of the platforms, the focus is on teaching at least the unit cells, with the BCC, FCC, and HCP type being the most treated. Furthermore, IVR technology has been used almost as much as NIVR (three platforms use the first, four use the second, and two use both (Figure 2)), while AR has been used on three platforms. Finally, it is observed that eight of the 12 analyzed works include some type of study to evaluate the training effectiveness of the platform or to find out the opinion of the students.

Still, the main virtual laboratories dealing with this topic in the last years are described in this paper. Given the limited evidence of the use of these new technologies (VR and AR) in the field of crystallography, authors consider that the potential of such technologies is being little exploited in the education sector. On many occasions, it may be because to design this type of VRLE, a multidisciplinary team is necessary in which some dominate the knowledge of the subject (in this case, crystal lattices) and others the programming and development part in VR or AR. Nonetheless, these technologies are being used every day in more sectors (medicine, engineering, biology, education, etc.) given that, in many cases, they solve difficult situations facing other resources: space, cost, danger associated to certain experiments, etc. [57,58]. In the case of crystal lattices, the main problem that the VR or AR can solve is the spatial comprehension, since not only does the student have difficulties in spatially understanding these concepts, but the instructor may also have difficulties in explaining crystallographic networks if they do not have some didactic resource for it. In this sense, the authors' experience using the VRLE presented in this paper in the classroom is satisfactory for both the instructor and the students, which corroborates the experiences evaluated in previous works in this same sector [40–52].

6. Conclusions

In this article, a systematic literature review (SLR) has been carried out to check which applications based on virtual reality (VR) or augmented reality (AR), both virtual reality learning environments (VRLEs), have been developed to date in the academic field to support the teaching of concepts related to crystallography. The results obtained by the SLR allow to observe that, despite the current expansion of both VR and AR in many fields, in the environment of crystallography teaching, there are still few works carried out with these technologies. Likewise, within crystallography, it can be seen that projects based on both immersive VR and non-immersive VR have been practically the same, with AR being the least used technology so far. Despite the limited expansion of VR and AR technologies in the educational field of crystallography, surely due to the difficulty of having a multidisciplinary team to carry out the design of a VRLE, all the experiences reflected in the SLR presented in this article are positive since VRLEs help both instructors and students to better face the problems of spatial vision in the teaching-learning process of crystallographic networks. As technology continues to advance, future efforts are needed in developing further interactivity and to reduce the cost to make these systems more accessible, as well as in expanding different and easy-to-use teaching tools (e.g., e-books, in the cloud, etc.) for enhanced implementation in the class and curriculum development.

Supplementary Materials: The following are available online at http://www.mdpi.com/2073-4352/10/6/456/s1, Video S1: Virtual and Augmented Reality Environments to Learn the Fundamentals of Crystallography—Demonstration of User Experience.

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Nomenclature

AR	Augmented Reality
BCC	Body-centered Cubic
CAVE	Cave Automatic Virtual Environment
CCDC	Cambridge Crystallographic Data Center
COD	Crystallography Open Database
DC	Diamond Cubic
FCC	Face-centered Cubic
HCP	Hexagonal Close-packed
HMD	Head-mounted Display
ICT	Information and Communications Technology
IVR	Immersive Virtual Reality
MEMS	Micro-electro-mechanical Systems
NIVR	Non-immersive Virtual Reality
PC	Personal Computer
SLR	Systematic Literature Review
SMA	Shape Memory Alloy
STEM	Science, Technology, Engineering and Mathematics
TEM	Transmission Electron Microscope
UE4	Unreal Engine 4®
VR	Virtual Reality
VRLE	Virtual Reality Learning Environment
WOS	Web of Science

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