“Virtual PVD”: A Virtual Reality approach to explore PVD Magnetron sputtering

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Abstract. The physical Vapor Deposition (PVD) surface treatment process consists of numerous steps involving of multi-physical and multi-scale phenomena. These phenomena are beyond the ability of human perception in their entirety which is a scientific challenge for learning PVD. The present article proposes a Virtual Reality (VR) approach dedicated to the PVD process learning and a prototype is developed with different modules. The virtual immersion includes two modalities. One *ex-situ*, in the surface treatment laboratory, at a real scale (1:1), allowing users to explore the process, the machine components, and to experiment with technical gestures such as handling the machine door or installing substrate-holder rods inside. The second modality is *in-situ*, enabling the user to follow the process steps immersed in an environment inaccessible to humans and multi-scale. These experiments help to understand the physical phenomena occurring throughout the deposition process (pumping, visualization of atoms and molecules, plasma, sputtering, and growth). The data feeding the application comes from measurements from the real system as well as from numerical simulations.

Keywords: Physical vapor deposition (PVD), Numerical simulation, Virtual reality (VR), human-machine interaction.

1 Introduction

1.1 Context

Physical Vapor Deposition (PVD) is a vacuum surface treatment process, commonly used in industry and research laboratories. It involves adding a thin layer (between a few nm and a few µm) of material to the surface of a part to modify its properties (tribological, mechanical, electrical, magnetic, optical, chemical, biological, etc.) [1].

The treatment is carried out in a chamber maintained under vacuum (0.0001 to 1 Pa) by a pumping system. It consists of transporting a metal vapor, in either a reactive or non-reactive atmosphere, from one or more sources to the substrates (the parts to be coated), where the vapor ultimately condenses, nucleates, and grows to form a film.

There are two main types of physical vapor deposition processes: evaporation and sputtering. In both cases, the process involves three steps: vapor creation, transport, and growth. The main difference that allows them to be classified this way lies in the generation of the vapor. However, it is worth noting that, due to the differences in the energy of the fluxes [2], the properties of the films obtained will also be different.

- The evaporation process involves heating the metal to its melting point so that it evaporates, using various techniques: Joule effect, induction, electron bombardment, electric arc. The working pressure is low (around 10^{-4} Pa), and the energy of the species is generally low (around 0.1 eV), except for the arc (around 50 eV).
- Sputtering relies on the mechanical effect associated with ion bombardment. The ion flux is generally obtained by a glow discharge plasma, which implies a higher working pressure (around 10^{-1} Pa) than evaporation. The species are also more energetic (around (eV). It is worth noting the particular case of ion beam sputtering, which uses an ion gun and can therefore operate at low pressure.

In this paper, the proposed "Virtual PVD" platform focuses on magnetron sputtering with plasma, but can be extended to other techniques.

1.2 Problematic

The illustration of PVD process in the context of teaching and training presents challenges. The physical principles involved and the technical processes can be relatively conceptual and difficult for learners to understand and visualize. The equipment used for PVD is often complex and expensive (pumps, power generators, sensors, actuators, etc.). Moreover, PVD involves phenomena that occur at the atomic or molecular scale and are therefore not directly observable to the naked eye.

To overcome these difficulties, this project proposes using immersive and interactive digital technologies, such as Virtual Reality (VR), to train professionals and students in a safe, economic, ecological, and interactive manner. The VR application will allow them to explore and understand the theoretical and practical aspects of the PVD process while providing an engaging and accessible learning experience.

The main challenge lies in the realistic, usable, and comprehensible visual representation of the phenomena that occur during the PVD process. It involves reproducing realistically the phenomena, such as material evaporation, atom transport in the vacuum chamber, and condensation on the substrate, adapting the scale and density of the atomic particles for the visibility and usability while ensuring a visualization experience faithful to the actual PVD process. Since these phenomena are normally invisible to the human eyes, another challenge is to design interaction and visualization metaphor allowing human to perceive and interact with them in the virtual environment.

This article is organized as follows: Section 2 reviews the related work providing an overview of using eXtended Reality (XR) to help learning invisible phenomena in the literature. Section 3 outlines the proposed approach, detailing the methodology and theoretical framework. Sections 4 and 5 describes the prototyped solution, including design and implementation details. Finally, Section 6 concludes the article, summarizing the findings and suggesting directions for future research.

2 Related works

2.1 Dedicated to material science

Achuthan *et al.* present how the use of computer techniques, such as enhanced multimedia simulations and interactive animations, can help students better understand invisible physical phenomena [3]. The study was conducted with engineering students and compared learning outcomes between traditional classroom teaching, real laboratory experiments, and virtual laboratories. It showed that traditional methods had significant limitations, while the approach combining classroom teaching with virtual laboratories had a positive impact on students' visual and conceptual understanding.

Sotiriou *et al.* demonstrate how the use of Augmented Reality (AR) in science education increases students' intrinsic motivation and cognitive learning of invisible physical phenomena in science [4]. The combination of classroom teaching and the AR approach seems to have a significant impact on students' understanding.

Virtual Reality (VR) technologies allow the illustration of phenomena invisible to the human eye in reality and the conduct of scientific experiments in the virtual world in materials science [5]. Virtual immersion allows learners to be transported into the world of the infinitely small, where phenomena occur at the atomic scale. This confirms the interest in using VR in the context of PVD, as it addresses similar issues.

2.2 Dedicated to PVD

A VR application was developed for the D.A.U.M. platform (Deposition and Analysis in Ultra-vacuum for nano-Material). The aim of this "Virtual D.A.U.M." is to allow the public conducting experiments in the laboratory as a scientific researcher. The scenario involves the creation of magnetic sensors and allows the sharing of the researcher's scientific approach, explains the laboratory's high-tech equipment, and gives meaning to concepts such as nanometric layers, single crystals, ultra-high vacuum, etc. [6]. But it is not specifically dedicated to the physics of the PVD process.

International coating companies (Hauzer, Plansee, and Von Ardenne) shared commercial videos explaining the general purpose of PVD and illustrating some of the physical phenomena [7, 8, 9]. But these videos are simply artwork without any interaction or immersion.

"VirtualPVD", a commercial simulation software, is proposed by Kurt J. Lesker [10]. It provides to customers 3D interactive views of the PVD process with some of the deposition parameters, such as deposition rate and thickness profiles. The aim is to assist users in the design and prediction of deposition outcomes, optimize processes, and design novel architectures. This software is not available for the public and moreover not dedicated to learn the PVD process.

In 2003, John C. Bean, launched "Virtual Lab" a website with videos and 3D models of molecules. A section was initially dedicated to PVD deposition [11], but unfortunately, it was not further developed.

These examples highlight the need of a comprehensive and scientifically-based virtual application for PVD, as proposed in this paper.

3 Proposed approach

In this article, a general framework of "Virtual PVD" application to illustrate and experiment with the magnetron sputtering deposition process is presented. Fig. 1 shows the available data flows and interactions between the user and the data, according to the usual paths (experimental or digital) and with the "Virtual PVD" application.

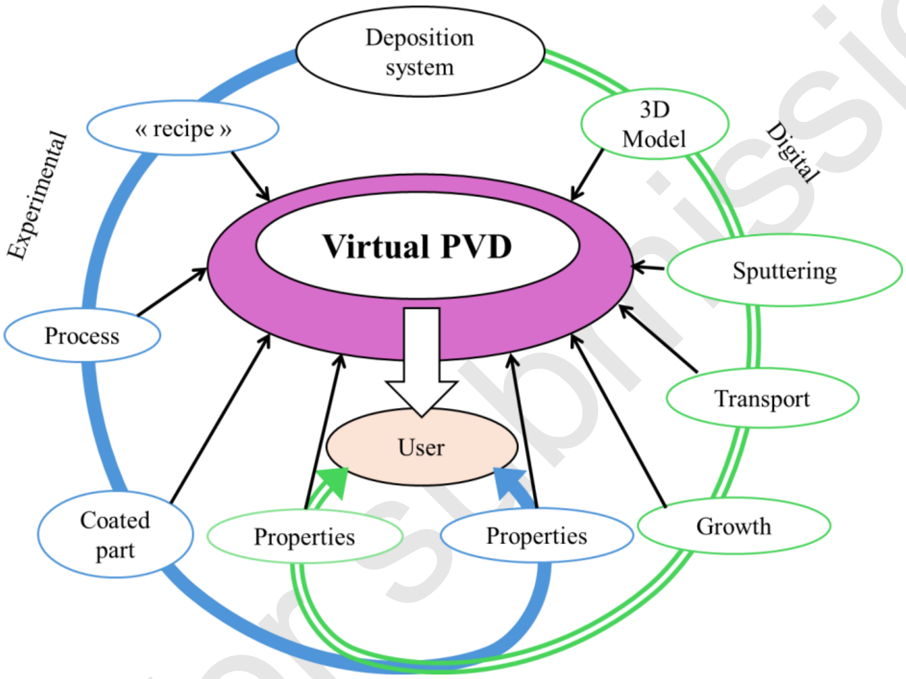

Fig. 1. Interactions between data from physical experiments and digital simulation and the user via the "Virtual PVD" application.

The experimental path (blue path in Fig. 1) is the most common, both in industry and in academy: it starts from a given deposition system and sequentially goes through all the steps from using a "recipe" to obtain the coated part and its characterizations. The digital path (green path in Fig. 1), actually more used in academy than in industry, involves using a 3D model of the chamber and software that sequentially simulates the three steps of the process: SRIM [12] for ejection, SIMTRA [13] for transport, and Virtual Coater© NASCAM [14] for growth and film properties.

In either path (or ideally both simultaneously), the user can only process part of the produced information, assuming it has already been collected. The quantity and heterogeneity (text, images, etc.) of this data make it difficult to fully comprehend. This is where the "Virtual PVD" application comes in, serving as an interface between the user and this mass of data.

The advantages of VR for experimenting with PVD are, on the one hand, the visualization of physical phenomena invisible to the human eye and, on the other hand, the multi-scale adaptation of the user's avatar (virtual representation) and the objects in the environment. The experiments and learning objectives will concern different scales (unique human scale vs. multi-scales) and different types of training (technical vs. scientific). Two categories of the virtual universe have been identified in the “Virtual PVD” application: *ex-situ* and *in-situ* (**Fig. 2**).

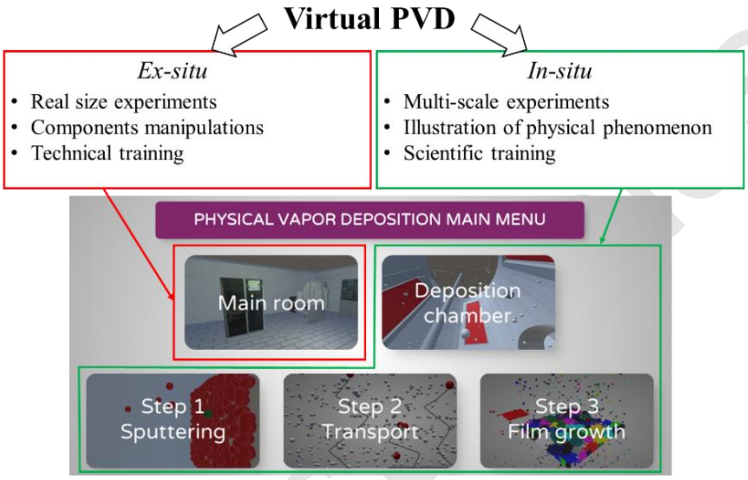

Fig. 2. Main menu of the “Virtual PVD” application with the two, *ex-situ* and *in-situ*, modules.

The main menu (**Fig. 2**) presents several virtual scenes: a “Main room” scene for *ex-situ* experience and several scenes for the different steps of the process for *in-situ* experiences.

In the ***ex-situ***, it is a virtual universe whose scale corresponds to that of the reality, as perceived by the user. For example, in a virtual tour of the PVD process workshop, the perceived space and the size of the virtual components correspond to real scales.

In contrast, the ***in-situ*** consists of a virtual universe whose entity scales are adapted to allow immersion and visualization. For example, in the real world a human can neither access the inside of a PVD machine due to its smaller size and the vacuum maintained inside, nor interact with molecules due to the scale incompatibility between the two. Whereas in the virtual world, the user avatar's size is reduced so that the user can enter and perceive the interior of the PVD chamber as a huge building (e.g., fig.7.a). The virtual molecules are enlarged so that the user can interact with them like balls.
These two categories of virtual scenes are detailed in the following sections.

4 Ex-situ scene: real PVD system usage conditions

In this module, real life scale and in a realistic environment with natural interactions with objects, are chosen. Two main functions are proposed:

- Navigation in the laboratory, exploring the deposition system, and discovering its various components: This function can be used for outreach to the non-scientific public as well as for general PVD training purposes aimed at technical and scientific audiences.
- Manipulating some components: This function allows for practice technical skills and gestures.

4.1 Discovery of the Deposition System

In this scene, the users find themselves in the laboratory where the deposition system is located (**Fig. 3**).

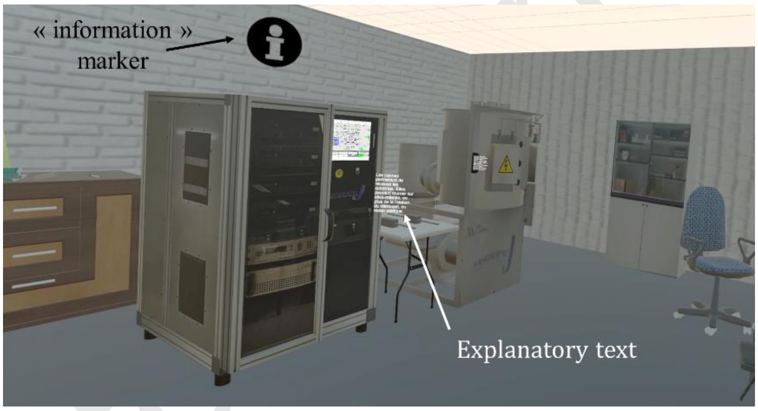

Fig. 3. The deposition system in its virtual environment.

The user can navigate in the virtual laboratory either through physical movements or by teleportation using game controllers. However, physical movements are limited by the real space where the user is located.

Markers (a black circle with an “i” visible at the top of **Fig. 3**) indicate places where information is available. This could be the description of a component (e.g., pumps, control and power board, acquisition systems) or the explanation of an action to be performed (e.g., opening the door). In order to minimize the number of markers that may disrupt immersion experience, only markers in the central field of view appear in the scene.

This virtual discovery is done without any risk (electrical, thermal, mechanical), without noise disturbance, and without disrupting the real system (for example, opening the door, which would stop the ongoing process and break the vacuum).

4.2 Manipulation of System Components

Taking advantage of the same benefits described above, the user can practice technical gestures (**Fig. 4**).

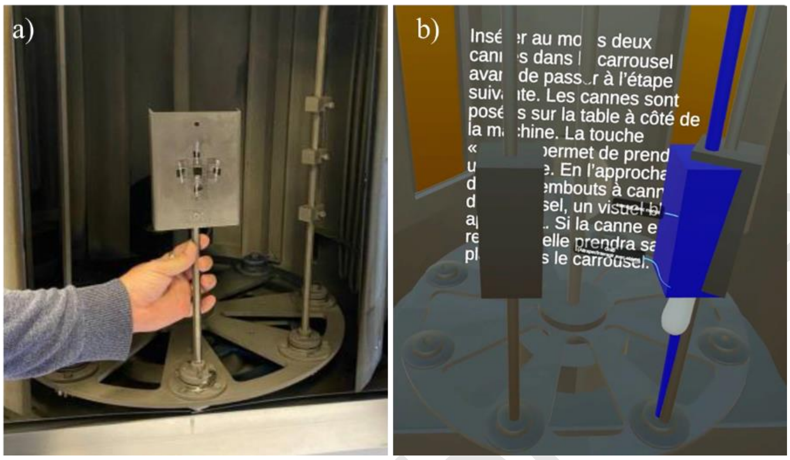

Fig. 4. Installation of a substrate holder rod: a) view of the real system; b) view in the "Virtual PVD" application.

In the current version of the prototyped "Virtual PVD" application, the user is invited to set up two substrate-holder rods in the carousel, which can hold up to eight. The carousel rotates around its central axis and each rod can also rotate around its own axis. The second rotation is allowed by a gear that can be connected to the static wheel located beneath the carousel. The substrates have to be fixed onto the rods outside the chamber, and then the rods are installed on the carousel. For that, a part containing a bearing and fixed with four screws to the upper part of the carousel has to be disassembled. All these operations take time and increase the risk of contamination of the chamber, due to the venting process and potential inadequate cleaning of the parts, or manipulation without clean gloves.

The advantage of training in this technical gesture virtually is that it does not require direct intervention on the real system. This allows for training without disrupting ongoing production or simply without contaminating the vacuum of the chamber by exposing it to the atmosphere for an extended period. Generally, the application allows for both in-person and remote presentations and training.

5 In-situ scene: multi-scale immersion

In this module, the “human” paradigm, meaning life-size and in a realistic environment with natural interactions with objects, is abandoned in favor of multi-scale immersion. The user has an unrealistic size relatively to the scale of the real system, ranging from a few centimeters to a few tens of centimeters. He is immersed in an environment naturally inaccessible to humans, namely the vacuum, and gravity is not always respected (the user is always standing on a horizontal surface, but this surface may not be physically horizontal in the real system). He can interact with physical entities (molecules and atoms) that are not visible to the naked eye: the dimensions of these entities, normally on the order of nanometers, have been enlarged to a few centimeters relative to the user's reduced size. For visualization comfort and computational power reasons, their number is significantly reduced to about a hundred units at a time.

The objective of this module is to visualize the steps of the deposition process and the physical phenomena occurring:

- Pumping of the initial atmosphere,
- Injection of working gas (Argon),
- Creation of plasma,
- Sputtering of the target,
- Transport of the sputtered atoms to the substrate,
- Film growth on the substrate,
- Film properties.

All these phenomena should ultimately be based on physical laws and data from process instrumentation and simulations of the different steps. At this stage of the development of the “Virtual PVD” application, only some data come from these two sources, but most phenomena follow simple physical laws integrated into the application.

5.1 Process progress monitor

To guide the user and allow him to “control” the deposition system, a tablet can appear on the left controller (**Fig. 5**).

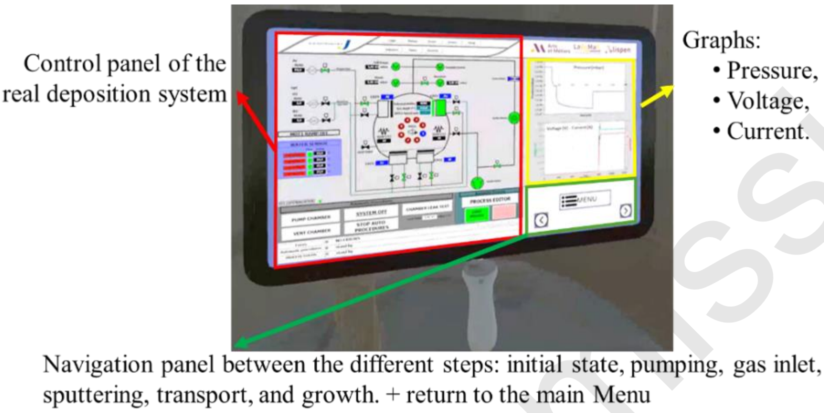

Fig. 5. Control tablet.

This tablet is used as a remote-control panel. It includes:

- The control panel of the real system with the different components (e.g., pumps, valves, gas mass flow maters, pressure gauge, heater, carousel, targets end their shutter), control parameters (e.g., gas flow and working pressure, temperature, rotation speed, electrical power), safety features (water flow, water temperature), etc.
- Graphs illustrating the process parameters over time (pressure, discharge voltage, current). This feature does not exist in the real control panel but allows for more direct process monitoring.
- A navigation panel that allows moving from one step to another and returning to the main menu (**Fig. 2**).

At each step, the values of the control parameters, the status indicators of the system components, and the graphs change. This tablet is also available in the main laboratory scene.

5.2 Visualization of the atmospheric particles

Different atmospheres will be encountered during the process:

- At atmospheric pressure (10^5 Pa), during sample loading and unloading operations and in the initial moments of pumping, the gaseous species present are those of air (i.e., dioxygen O_2, dinitrogen N_2, argon Ar, carbon dioxide CO_2, methane CH_4, and water vapor H_2O).
- Once the pumping (primary pumping followed by secondary pumping) is completed, the residual vacuum (around 10^{-4} Pa) is reached, and only a few large molecules and gas atoms remain.
- During the entire deposition process, the working pressure is on the order of 10^{-1} Pa. The atmosphere mainly consists of argon (in both neutral and ionized forms), possibly reactive gases (O_2, N_2), and sputtered metallic species from the target.

The atmosphere in the chamber is represented by gas molecules and atoms, enlarged to be visible (**Fig. 6**). As a result, their number is significantly reduced, and theoretical proportions (e.g., for air: 99 % for O_2 and N_2 and 1 % for all the remaining gas) are not respected to visualize contaminant molecules present in a few ppm. The atoms and molecules exhibit random behavior in the chamber with elastic collisions between them and with the walls. Adsorption, desorption, and combination phenomena are not yet represented.

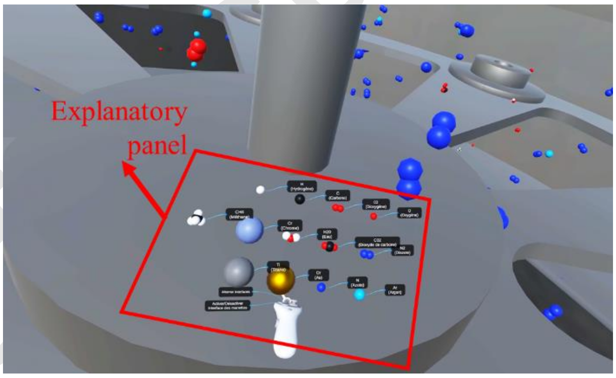

Fig. 6. Gas molecules and atoms in the atmosphere and explanatory panel.

To help the users to identify the atoms and molecules, an explanatory panel (**Fig. 6**) can appear above the controller. The molecules and atoms are organized in a grid with a small label indicating their name. The user can follow the molecule of interest with their hand while viewing the descriptions through the transparency of the grid.

The gas molecules respect the bonding angles (180, 120, or 109.5°) [15] and the size of the atoms is proportional to their atomic radius [16]. The color code, based on the CPK (Corey-Pauling-Koltun) model [17, 18], is the one proposed by the Jmol software [19] as it covers the entire periodic table of elements.

5.3 Visualization of the sputtering

Sputtering is achieved through the presence of plasma, the fourth state of matter. It is what truly defines this deposition process. The plasma is here a glow discharge created and maintained by operating above a certain pressure and applying electrical power to the targets. It generates ions that sputter the targets and produce the metal vapor, which redeposits onto the substrates to form the film. Plasma can also be used to clean the substrates and densify the growing layers. Plasma is a gaseous mixture, globally electrically neutral, consisting of neutral atoms, ions, and electrons. The de-excitation of ions emits photons whose frequencies are characteristic of the elements involved, allowing the process to be monitored through the emitted optical spectra. To increase deposition rates, the plasma is confined by a magnetic field near the targets, giving it a typical toroidal appearance.

In the "Virtual PVD" application, two scales are represented simultaneously (**Fig. 7** a and b).

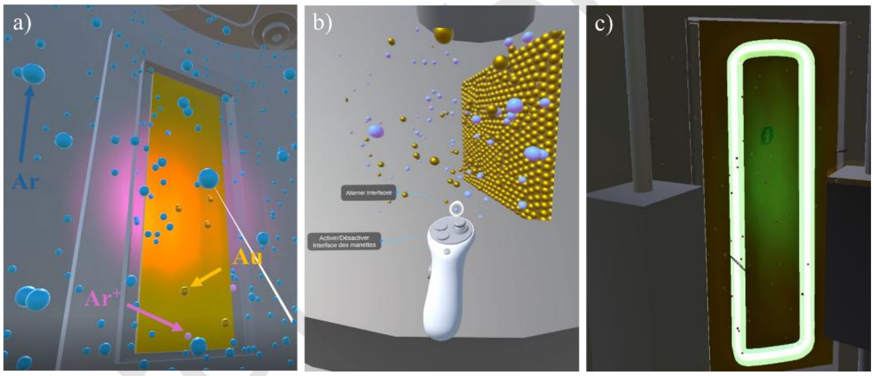

Fig. 7. Visualization of plasma: a) illustration of species involved in plasma; b) zoom on sputtering; c) visualization of more realistic plasma from the main room.

First, the user is in the chamber, at the stage where he has injected argon to reach the working pressure, and he visualize the argon atoms (**Fig. 7**.a). When an atom passes near the surface of a target, it is captured by the electric field, loses an electron to become an Ar^+ ion, and is attracted to the negatively polarized target. Due to multiple collisions in matter, surface atoms from the target are ejected. These phenomena can be visualized with an atomic-scale zoom above the controller (**Fig. 7**.b). Second, a glow near the target appears to represent the photonic emission. However, this plasma representation in **Fig. 7**.a is not realistic. A dedicated scene (**Fig. 7**.c) for plasma has been developed as an independent module. This scene allows visualizing the color and intensity of the photonic emission based on process parameters: working pressure, power applied to the targets, nature of the species (metallic and gaseous).

Due to the sputtering, the target is progressively worn and a “racetrack” is observed. It corresponds to the maximum intensity of the plasma confined by the magnetic field. In a dedicated scene, the user can walk virtually on the target (**Fig. 8**).

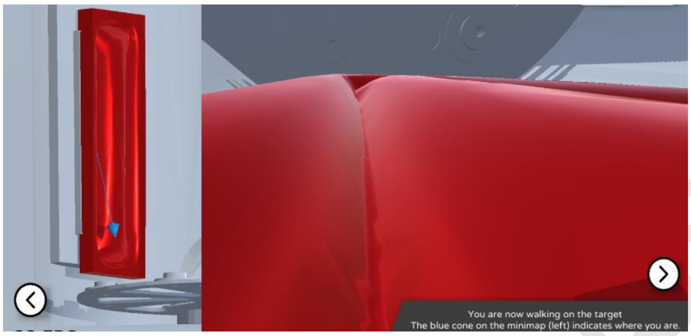

Fig. 8. Visualization of the racetrack.

The mini-map on the left side of **Fig. 8** shows the position (blue “eye”) and the looking direction (blue ray) of the avatar on the target in the chamber reference frame. On the right, the first person view of the user on the target topography is illustrated.

5.4 Visualization of the transport

To visualize transport, the user is positioned to the top of one of the two substrate holder rods that were installed into the chamber in the main room scene (**Fig. 9**).

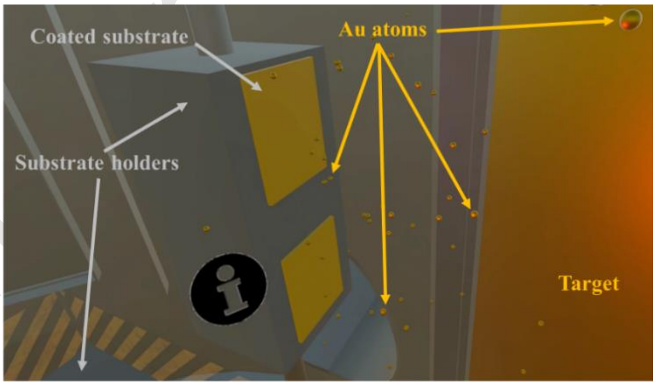

Fig. 9. Visualization of atom transport from the target to the substrate.

The user can move on this platform within the limits defined by virtual barriers. This safety feature is essential for users comfort, as they find themselves at a height and may be disturbed by the void in front of them. From this platform, they see metal atoms leaving the target, changing trajectory due to collisions with gas atoms, and reaching solid surfaces (including the substrate). Gradually, the substrate changes color to illustrate the film formation.

5.5 Visualization of the growth

The final scene allows visualizing film growth on the substrate at the atomic scale. **Fig. 10**.a represents the beginning of the columnar film growth with the formation of the first clusters on the substrate. The colors of the atoms represent the columns they belong to.

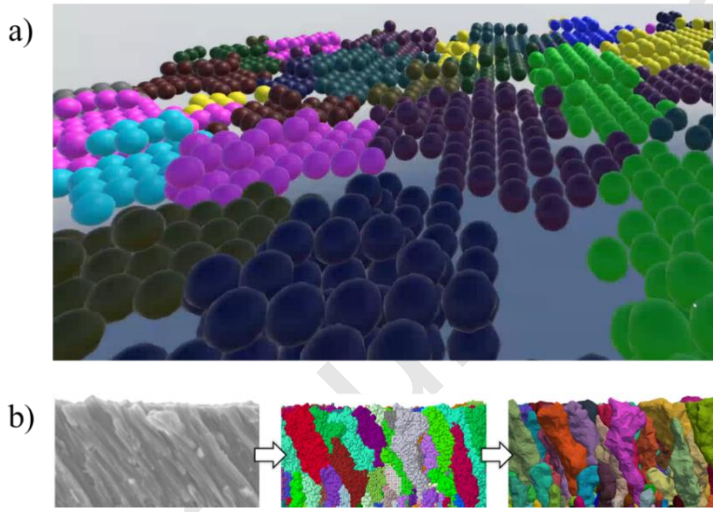

Fig. 10. Film growth: a) atomic view; b) columnar view [20].

In this visualization, the atoms all have the same atomic radius and are placed on a cubic grid. The coordinates and order of arrival of the atoms come from numerical simulation [14]. The atoms are deposited on the substrate with a straight trajectory, representing only the direct path following the last collision. The user can observe from outside of the columnar film or go among the atoms and immerse himself in the growing film. However, he cannot disrupt the structure by moving the atoms by hand.

The columnar microstructure of the film at the end of the deposition process can also be represented (**Fig. 10**.b). The point clouds of entire columns, derived from clusters, are individually meshed [20] and correspond to the real microstructure. The use of colors again serves to differentiate the columns from each other.

6 Conclusion and perspectives

In this article, a virtual reality application dedicated to the PVD vacuum process was proposed. The prototype includes two modes. One is *ex-situ*, in the surface processing laboratory, at real-size, allowing the discovery of the process and the machine components, as well as technical gesture experiments such as manipulating the door or setting up substrate holder rods. The second is *in-situ*, allowing the user to follow the process steps in an environment inaccessible to humans and at multiple scales. These experiments help understand the physical phenomena occurring throughout the deposition process (pumping, visualization of atoms and molecules, plasma, sputtering, transport and growth). The data feeding the application comes from measurements obtained from the real system as well as numerical simulations. Significant work remains to integrate a larger volume of this data.

There are also many scenarios to develop in terms of training and experiments: for example, maintenance operations on the targets, visualization of pump technology operations, visualization of material flow distribution, or even film properties in the chamber based on process parameters, visualization of plasma characteristics based on deposition parameters, etc.

One of the most interesting perspectives of this "Virtual PVD" solution is the integration of data flow (from experimental instrumentation and numerical simulation). Using the augmented reality modality, this would assist interventions on the PVD system by overlaying all necessary virtual information onto the real environment. Another perspective is using immersive virtual reality as teleoperation user interface to allow remotely controlling the real system. User could see the digital twin of the real system and detailed virtual information of the process.

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