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INTERACTIVE VIRTUAL COMPARISON OF PURE AND ALLOY CRYSTAL STRUCTURES IN MATERIAL SCIENCE LESSONS

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Abstract:

Visualizing something invisible to the naked eye, such as the crystal structure of a material, presents a significant challenge in understanding the field of material science. Thus, this project aims to develop an augmented reality (AR) mobile application that can visualize and compare the crystal structure of pure and alloy metals to assist in understanding material science. AR is used to integrate real-world data with computer-generated content to provide an interactive approach that goes beyond traditional methods. The models of the crystal structures are generated using SolidWorks software and then integrated into Unity software to blend the structure into the real-world application. Next, Vuforia software is used to make AR accessible on mobile phones. As a result, 'Crystal View 1.0' is developed and ready to use on students' smartphones. The application offers a mixed reality view, enabling the real-time visualization of the crystal structures and detailed descriptions. 81% of mechanical engineering students taking material science courses are interested in using AR to learn crystal structure. In conclusion, the application can help students visualize and differentiate the crystal structures of pure and alloy metals interactively with real-world applications, thereby boosting the motivation of science students to learn material science.

Keywords:

Augmented Reality, Crystal Structure, Education, Material Science

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Introduction

Material science is an important discipline that focuses on studying materials' properties, structure, and performance. Understanding material science is crucial in various industries including design, architecture, engineering, and manufacturing. One of the fundamental studies of material science is the concept of crystal structures. Crystallography is the study of the specific arrangement of atoms, ions, or molecules in a repeating pattern such as cubic, tetragonal, or hexagonal for a specific material. Figure 1 shows the 14 Bravais lattices as fundamental for the crystal structure of crystalline materials. These arrangements determine a material's properties. For example, the hexagonal crystal structure of titanium has higher tensile strength and rigidity than aluminium's cubic crystal structure.

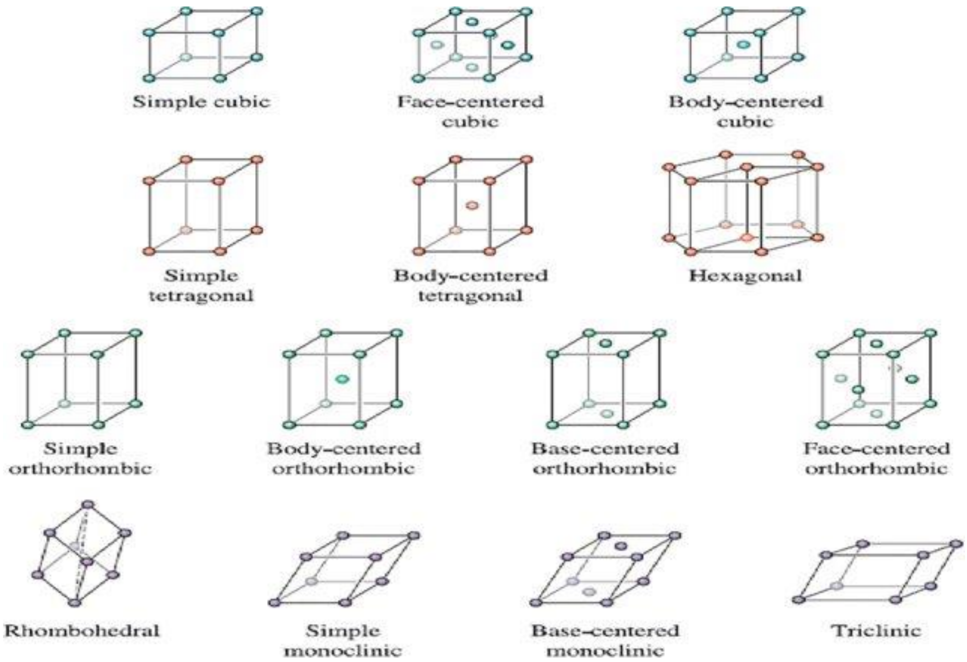

Figure 1: The 14 Bravais Lattices

Source: (Askeland et al. 2021)

However, visualization and comprehension of these arrangements often present significant challenges since crystal structures exist on the atomic level, millions of times smaller than the width of a human hair, making them invisible to the naked eye. The crystal structures are inherently abstract concepts, making it difficult for students to form a mental model of the structure. Usually, traditional methods such as blackboard teaching, slides, and physical models have been employed in teaching crystallography (Horikoshi et al., 2021; Wang & Liu, 2023). However, these methods pose limitations in terms of 3D visualization and interactivity. Physical models, although helpful for visualization, lack feedback and dynamic interaction with real-world applications. This lack of interactivity and connection to real-world applications can hinder students' ability to fully grasp the relevance and significance of crystal structures in various fields.

In addition, certain crystal structures, such as metal alloys, present further challenges. These structures involve complex arrangements of different elements or atoms as shown in Figure 2,

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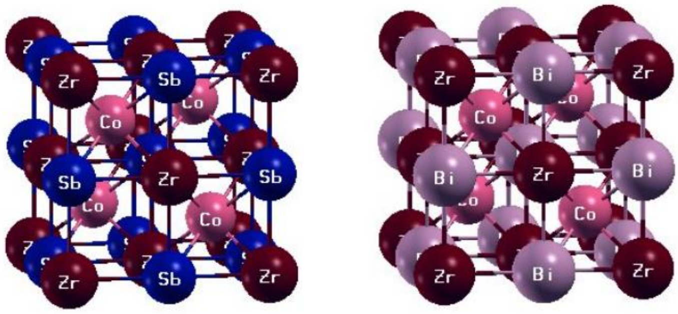
which can be interstitial (smaller atoms occupying spaces between larger atoms) or substitutional (atoms of one element replacing those of another). The varying sizes and positions of atoms in alloys make them more difficult to visualize and understand compared to pure metals or single-element crystals.



(a) (b)

Figure 2: The Crystal Structure of Half Heusler Alloys (a) ZrCoSb and (b) ZrCoBi
Source: (Allan et al., 2022)

Since traditional teaching methods have visual and interactive limitations, virtual reality (VR) and mixed reality technologies like augmented reality (AR) offer solutions for these problems. While there have been numerous studies exploring the use of AR and VR for education, there is a lack of research focusing on the specific visualization and comprehension of metal alloys commonly used in engineering, such as steel, brass, and bronze (Rebello et al., 2024; Extremera et al., 2022;Mazzuco et al., 2022). VR provides fully immersive experiences in simulated environments, it often requires specialized equipment and may not be accessible to all learners. AR, on the other hand, leverages readily available devices like smartphones and tablets to seamlessly blend the real world with interactive 3D visualizations.

Therefore, AR has significant potential in this context. By creating interactive 3D visualizations of crystal structures, AR can bridge the gap between the microscopic world and our human perception, allowing for a deeper understanding of these fundamental building blocks of pure and alloy. Nechypurenko's 2018 study indicated that there was no use of real objects as markers in augmented reality applications for crystal structure learning. To date, this trend appears to continue, with the literature review revealing no evidence of the use of real objects or real-world applications that integrate crystal structure learning with the students' physical environment. This limitation highlights a gap in the existing research, as the use of real-world objects as markers could potentially enhance the learning experience by providing a more tangible and interactive way to visualize crystal structures. Thus, this study aims to develop an AR mobile app using a marker from an image target and a modal target. Next is to investigate the efficiency of developed AR mobile applications in improving student motivation, visualization, and comprehension of crystal structure between pure and alloy metal. According to the scope purposes, the main research questions addressed by this paper are:

RQ1: Does the use of an AR mobile application with image and model targets lead to improvement in students' ability to differentiate between pure and alloy crystal structures compared to traditional teaching methods?

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RQ2: What are the perceptions of mechanical engineering students regarding the use of an AR mobile application with image and model targets for learning about crystal structures, and how does it impact their motivation and engagement in material science courses?

Literature Review

This section focuses on the importance of visualizing crystal structures, interactive learning of AR in education, and interactive learning aids for crystal structures.

Importance of Visualizing Crystal Structure

Crystal Structure is a critical factor in influencing the material properties, such as the presence of dislocation. Dislocations a defect within the crystal lattice, can significantly impact both the ductility and the strength of the material. Wen et al. (2022) highlights the importance of visualizing crystal structures to understand complex transformations. Their study investigated the effect of stress and thermal on the crystal structure changes in a titanium-aluminium alloy. These changes involved a transformation from face-cantered cubic (FCC) to hexagonal closed pack (HCP) to face-cantered tetragonal (FCT) crystal structure. To understand the effect of the transformation on the alloy, the researchers use an open-source software called OVITO to analyse the atomic position, grain boundaries, and dislocation.

Visualizing these complex atomic arrangements is crucial for understanding material behaviour at different scales. This ability to visualize and manipulate structures in 3D is a key skill for researchers in material science. Interestingly, research by Korakakis et al. (2012) suggests that students aged between 17 and 18 years old learn more science effectively in a 3D environment compared to younger students. This improved learning is attributed to the full development of crucial skills, such as metacognitive, spatial ability, and visualization skills. These findings highlight the potential of 3D visualization tools to enhance the understanding of complex concepts like crystal structure.

Interactive Learning of AR in Education

Beyond traditional educational methods, researchers are investigating the use of AR to facilitate learning in various fields such as sociocultural systems, medical, and engineering.

AR in Culture, Social, and History

Li et al. (2023) investigated the use of AR to improve social interaction and increase emotional expression for children with autism spectrum disorder (ASD). The study showed that the children could replicate the virtual agent's facial expressions and demonstrated greater independent learning compared to the traditional 2D methods. These findings suggest that AR interventions may hold promise for developing social skills in children with ASD. Furthermore, AR technology is also being explored for its potential in cultural preservation. Maulana et al. (2023) explored how AR can introduce younger generations to traditional elements. Their study used a 3D representation of Sumba woven cloth displayed on an image in a provided catalogue. However, the researcher highlighted that the effectiveness of AR detection was influenced by factors like the device used, the distance between the image and camera, the angle, and the lighting condition. Building on the potential of AR in education, Blanco-Fernández et al. (2014) explored how AR technologies can create an immersive learning experience for historical events. Their study focused on the Battle of Thermopylae between the Persians and the Greeks. Users engaged in a simulated battle scenario using mobile devices and QR codes on the floor.

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However, the researchers recognized that AR alone might not be sufficient for a comprehensive learning experience. Therefore, their approach extended beyond just AR by incorporating social networking functionalities, a repository of multimedia content, and remote expertise. This highlights the potential of combining AR with other technologies to create more engaging and interactive learning environments.

AR in Medical

Dickey et al. (2016) explored the use of Google Glass, an AR headset to improve urological surgery and training. Their study found the application to be valuable for both trainees and faculty. Faculty preferred its potential as a proctoring tool, while trainees found it useful for educational purposes. Some limitations were identified in the study, such as concerns about over-reliance by surgeons. This could lead to situations where surgical decisions might not align with the information provided by the AR. Kurniawan et al. (2018) investigated the effectiveness of mobile AR applications in supporting anatomy learning for high school and medical students. Their application offers various views and layers of the human body, addressing the need for high-quality learning materials. Students responded with a positive experience with the app, finding the 3D models clear, easy to understand, and interactive. However, the study also identified limitations in the application's usability. These included a lack of user guidance for beginners, a lack of multimedia elements, and annotations written in complex language and not user-friendly interface.

AR in Engineering

Bakkiyaraj et al. (2021) studied the effectiveness of AR for students learning 3D printing skills. It compares three AR learning modes within a mobile application. The three modes are textual instructions, demonstration videos, and interactive 3D animation. The results demonstrate that AR, especially the latter mode, significantly improves learning compared to the traditional method. This suggests that learner-centric, interactive experiences within AR can be highly effective for acquiring practical skills like 3D printing. Grodotzki et al. (2023) investigated the potential of AR for manufacturing education using Microsoft HoloLens2. Their study focuses on the benefits of AR for independent machine exploration and overlaying information on real machines. Students found hand interaction with holograms intuitive for close interactions. However, long-distance interaction proved frustrating. These findings suggest that AR can create engaging learning environments by combining the real world with holograms. However, further research is needed on improving gesture-based interaction for long-distance manipulation.

Interactive Learning Aids for Crystal Structure

Interactive learning aids have emerged as promising tools for enhancing students' understanding of complex scientific concepts. Researchers have explored various interactive learning aids, including virtual reality (VR), didactic virtual tools (DVTs), mixed reality (MR), and augmented reality (AR) applications. Table 1 presents an overview of notable studies that have investigated the use of these tools for crystal structure visualization, highlighting the different learning aids employed, the types of crystal structures visualized, the use of markers, and the key focus of their studies.

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Table 1: Interactive Learning Aids in Crystal Structure

References	Learning Aid	Crystal Structure	Marker	Remark
Bejjarapu et al. (2024)	Virtual reality	General cubic structure	-	For finding Miller Indices, no specific metal was given
Laricheva and Ilikchyan (2023)	Virtual reality	Tetrahedral and hexagonal	-	Atom vibration in solid diamond and graphite, atomic structure, periodic table
Stella et al. (2023)	Virtual reality	Diamond	-	Diamond unit cell, boding, and Miller indices
Kumar et al. (2021)	Virtual reality	General cubic structure	-	General visualization SC, BCC, FCC,
Maksimenko et al. (2021)	Virtual reality	Not specified	-	The crystal structure for solid elements but more focus on atomic structures
Caro et al. (2018)	Virtual reality	General cubic structure and hexagonal	-	General visualization SC, BCC, FCC, diamond cubic, and HCP
Mansoor et al. (2018)	Mixed reality, Microsoft Hololens	General cubic structure and ceramic basic structure	-	SC, BCC, FCC, NaCl. CsCl and ZnS. No marker was used
Jie et al. (2021)	Mixed reality, AR	Mineral	-	Quartz, Amethyst, Tiger's eye, Emerald and Amazonite. No marker was used
Müssig et al. (2020)	Mixed reality, AR	Pure metal cubic and hexagonal structure	Pre-image	Visual arrangement crystal structure for Co, Au, Fe, Pb pure metal

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Sharma & Mishra (2019)	Mixed reality, AR	Not specified	-	Given the example NaCl crystal structure with focus capabilities in powder diffraction simulation and analysis, crystallographic calculations
Liou et al. (2016)	Mixed reality, AR	General cubic structure and hexagonal	Pre-image	Visualization general SC, BCC, FCC, diamond cubic, and HCP

While many studies explore using virtual reality (VR) for studying crystal structures, these approaches have limitations. While offering valuable learning experiences, VR often lacks a direct connection to real-world objects. Additionally, VR requires complex hardware setups compared to AR. The previous studies in using AR for understanding crystal structures are limited by their reliance on pre-existing images to trigger 3D crystal models for AR. Thus, reducing the flexibility of the AR experience. Additionally, the focus on general crystal structures without connecting them to real-world objects hinders the exploration of more complex arrangements, such as metal alloys, and limits understanding through real-world applications.

In conclusion, existing 3D visualization applications, while valuable for presenting crystal structures, lack features specifically designed for directly comparing pure and metal alloy structures. This gap highlights the need for the present study, which introduces the application of the "model target" functionality alongside the standard "image target" commonly used in AR applications. This combined approach has the potential to create a more effective and engaging learning experience for students to interactively compare pure and alloy crystal structures.

Methodology

This study employed a phenomenological qualitative research design to explore students' experiences and perceptions of using the Crystal View 1.0 application in enhancing mechanical engineering students' visualization and comprehension of pure and alloy crystal structures. The application was developed using SolidWorks for crystal structure modelling. Next, Polycam was used to capture real-world objects as a model target. When captured by the camera, this model target would trigger the display of the corresponding crystal structure. Meanwhile, to display the crystal structure on an image, a pre-existing image is used as the image target. Finally, Unity and Vuforia software were used to integrate the model target, image target, and crystal structure model to develop a mobile application called Crystal View 1.0. The process flow of the application development is shown in Figure 3 and Figure 4.

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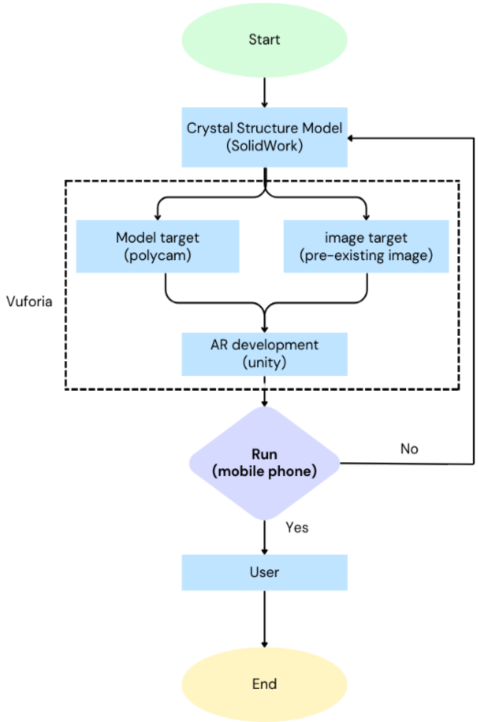

Figure 3: Augmented Reality Application Development

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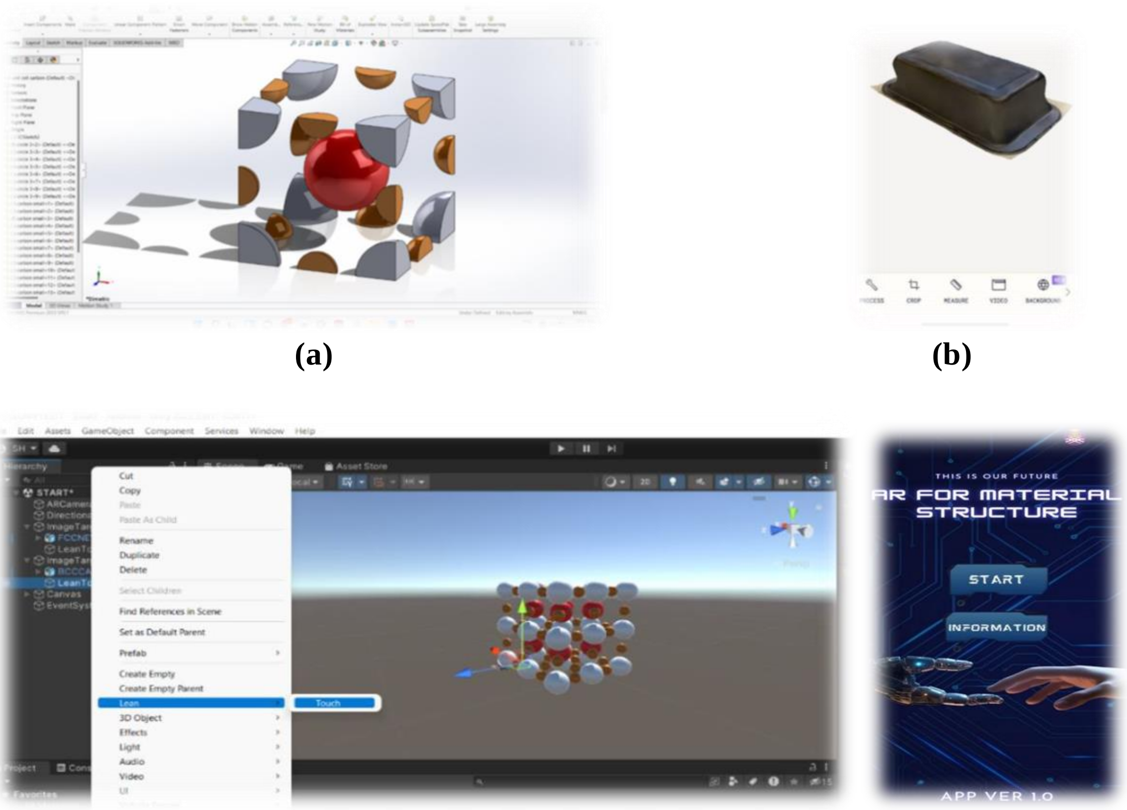

(a) (b)

(c) (d)

Figure 4: Model Target Development (a) SolidWorks Crystal Structure Model (b) Polycam Image of Real-World Object (c) Integration in Unity and Vuforia Engine and (d) Final Interface

Data were collected through an online questionnaire administered to 59 mechanical engineering students enrolled in material science courses (MEC281 and MEQ431) at UiTM Pulau Pinang to assess the level of visualization and comprehension of crystal structure. The survey consisted of open-ended questions aimed to gather qualitative data on student experiences, perceptions, and challenges related to understanding crystal structures.

The study was conducted in weeks 2 and 3 of the 14-week academic session from October 2023 to February 2024, as this topic is covered early in the syllabus. Survey responses were analyzed using thematic analysis to identify recurring themes and patterns in student feedback.

Results and Discussion

In this section, the AR mobile application called "Crystal View 1.0" is discussed, focusing on its features and effectiveness in enhancing crystal structure learning. The application was designed with these aims, incorporating features such as 3D visualization, real application detection, and detailed information on selected crystal structures. To ensure a smooth user experience, Crystal View 1.0 is designed to be compatible with smartphones that meet or exceed the specifications as shown in Table 2.

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Table 2: Smartphone Specification for The Crystal View 1.0

Specification	Minimum Requirement
Screen Size	6.4 inches
Resolution	720 x 1560 pixels
Operating System	Android 10
Sensor	Accelerometer
Ram	3 GB
CPU	1.8 GHz Octa-Core

The application has been specifically developed for Android smartphones, taking advantage of the platform's developer-friendly and open-source environment (Umar, 2023). Currently, the installation process involves downloading the APK file, however, the application is planned for future release on both the Google Play Store and the Apple App Store, offering a more convenient installation experience for a wider audience. Upon launching Crytal View 1.0, users are presented with a clear and intuitive main menu. This menu provides access to the core features of the application, including the option to select either an image target or a model target as shown in Figure 5.

Choosing the "model target" functionality allows users to view the crystal structure overlay directly on a real object. By pointing a smartphone camera at an object like an aluminium baking pan, the application can display the unit cell, the smallest unit for the crystal structure that the object represented, such as an FCC crystal structure as shown in Figure 6 (a). Meanwhile, Figure 6 (b) shows the "image target" functionality that displays the crystal structure overlay directly on a pre-existing 2D image of a carbon steel baking pan. A model target is a specific type of marker used for object recognition and tracking.

Figure 5: Crystal View 1.0 Application Interface

Unlike traditional image targets that typically use a flat image like a QR code or pre-existing images, model targets utilize 3D models. This unique feature in Crystal View 1.0 enables the ability to interact with virtual content directly on the physical object, creating a more immersive and engaging AR experience. In addition, model targets can be used with a wider range of objects, including those with complex shapes or non-planar surfaces.

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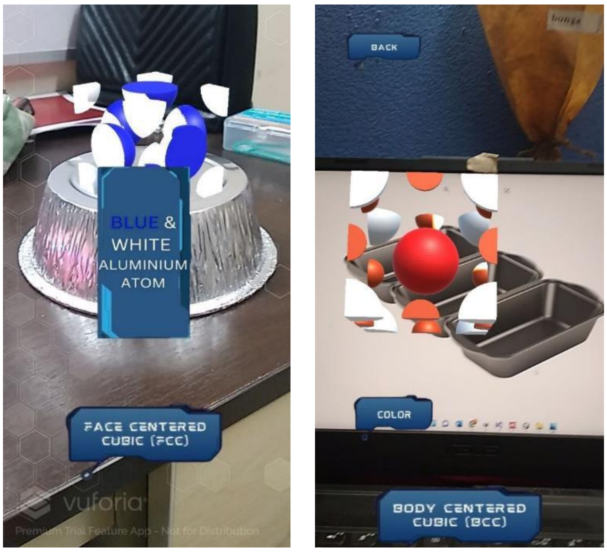

(a) **(b)**

Figure 6: Unit Cell Of (a) Pure Aluminium Using Model Target And (b) Alloy Metal (Steel) Using Image Target

In addition to visualizing crystal structures, Crystal View 1.0 includes an integrated colour-coding explanation feature. This feature helps users understand the colour scheme used to differentiate between atoms of the same type and those of different within the crystal structure. This allows users to distinguish the arrangement of atoms between pure and alloy metal crystal structures. Unlike pure metals, where all the atoms are the same size and tend to form very regular structures, alloy (Figure 7) shows multiple types of atoms with different sizes.

The yellow atom shows the position of carbon atoms that intersect between iron (white) atoms. The red atoms are the same size as the white ones indicating the same iron atoms but in different positions.

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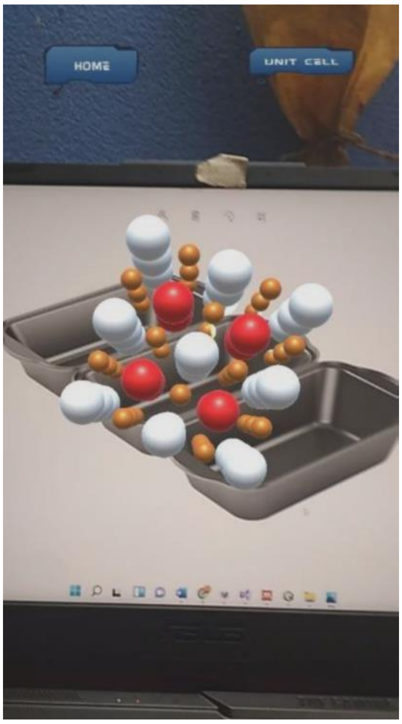

Figure 7: Crystal Structure of Steel with The Different Colour Coded for Different Atoms and Positions

The application also includes information related to the explanation of crystal structures, which can be updated periodically. This comprehensive approach makes Crystal View 1.0 a valuable one-stop reference for students. This application is simple yet effectively serves its purpose to help students visualize crystal structure. It is a more accessible alternative to virtual reality, which typically requires a complex setup and offers limited interaction with actual objects (Kumar et al., 2021).

The survey results as shown in Figure 8, indicate a strong student preference for using AR compared to the traditional method for learning and understanding crystal structures in material science. An overwhelming 81% of students expressed interest in using AR for this purpose. The students considered the experience of using AR to be interactive and motivating as expected from similar research findings (Garzón et al., 2019). Some of the students' feedback after using the application "This 3D crystal structure app is a winner, helps visual learners much faster than using a flat picture", "This application makes learning enjoyable" and "I can relate to the crystal structure with actual applications and differentiate between pure and alloy crystal structures".

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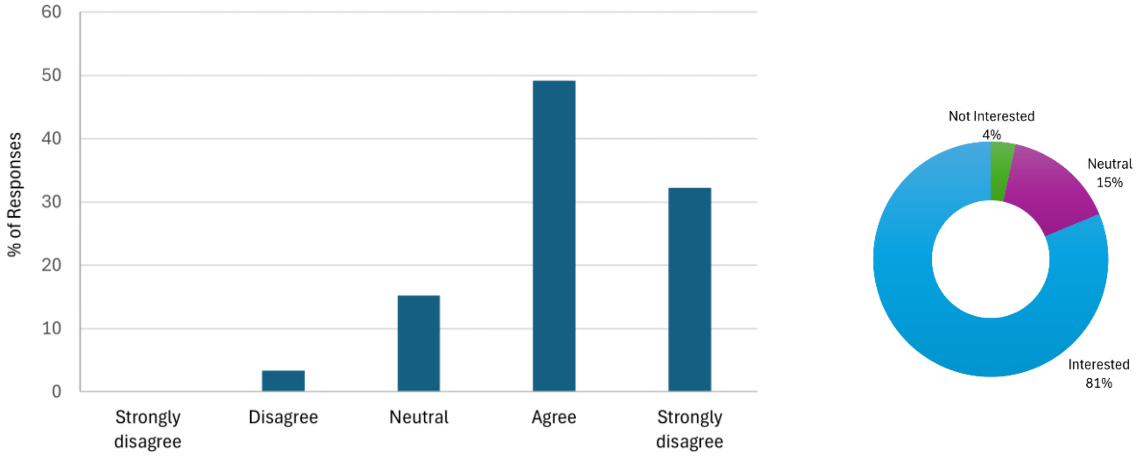

Figure 8: The Interest of Use AR vs Traditional Method

Based on Figure 9, students show significant level of comprehension in crystal structure for pure and alloy. This is because from the colour coded system that has been shown to the students, as can be seen in Figure 7. Additionally, the improvement in the visualization for the students might be because of they can zoom in and rotate the crystal structure to clearly see the individual atoms. By zooming in, students can focus on specific areas of crystal lattice and examine the atomic packing arrangements in detail. Student can see either the alloying element located in between or replacing parent atoms. Rotating the structure allows them to visualize the crystal from various angles, providing a more comprehensive understanding in 3D spatial direction. While the colour-coded system and other interactive features significantly enhance learning, incorporating animations that highlight the formation of crystal structures could further improve the comprehension in future.

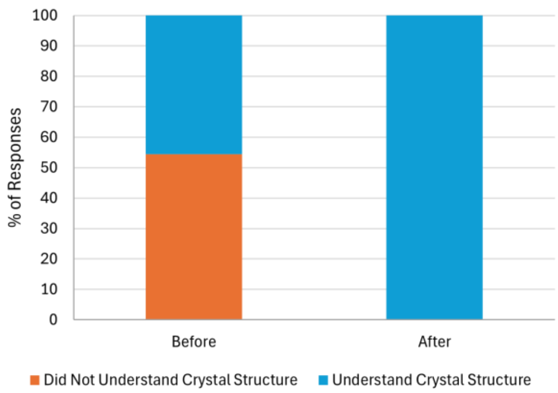

Figure 9: Effectiveness of AR Application in Visualize Pure and Alloy Crystal Structure

Conclusion

This study investigated the effectiveness of an augmented reality (AR) mobile application, Crystal View 1.0, in enhancing mechanical engineering students' understanding of crystal structures pure and metal alloy. The findings of this research offer valuable insights into the potential of AR as a learning tool in material science education.

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RQ1: Does The Use Of An AR Mobile Application With Image And Model Targets Lead To Improvement In Students' Ability To Differentiate Between Pure And Alloy Crystal Structures Compared To Traditional Teaching Methods?

The results of this study demonstrate that the Crystal View 1.0 application significantly improved students' ability to differentiate between pure and alloy crystal structures. The use of image and model targets, coupled with interactive 3D visualizations and color-coded representations, enabled students to grasp the differences in atomic arrangements more effectively than traditional 2D diagrams and physical models. This finding aligns with previous research highlighting the benefits of AR in visualizing complex scientific concepts.

RQ2: What Are The Perceptions Of Mechanical Engineering Students Regarding The Use Of An AR Mobile Application With Image And Model Targets For Learning About Crystal Structures, And How Does It Impact Their Motivation And Engagement In Material Science Courses?

The overwhelmingly positive feedback from students regarding the Crystal View 1.0 application underscores its potential to revolutionize the learning experience in material science. Students found the application to be engaging, motivating, and helpful in relating abstract crystal structures to real-world applications. This increased engagement and motivation can translate to improved learning outcomes and a deeper appreciation for the subject matter. The survey responses suggest that incorporating AR into material science courses could foster a more interactive and enjoyable learning environment, ultimately leading to a better understanding of fundamental concepts like crystallography.

Limitations and Future Directions

While the Crystal View 1.0 application has shown promising results, it is important to acknowledge its limitations. Currently, the application has a limited database of real-world objects and does not incorporate real-time material detection capabilities. Future development of the application could focus on expanding the database to include a wider variety of materials and integrating real-time detection to provide a more comprehensive and immersive learning experience.

In conclusion, the Crystal View 1.0 application successfully enhanced students' visualization and understanding of crystal structures, particularly in differentiating between pure and alloy metals. Furthermore, it garnered positive feedback from students, indicating its potential to increase engagement and motivation in learning. Future research could explore the long-term impact of AR on student learning outcomes and investigate its applicability in other areas of material science education, while addressing the limitations identified in this study.

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