A hands-on activity to introduce the structure of NV-center quantum bits in diamond

Ockhorst, R.; Koopman, L.; Pols, C.F.J.

DOI
10.1088/1361-6552/ad4765

Publication date
2024

Document Version
Final published version

Published in
Physics Education

Citation (APA)
Ockhorst, R., Koopman, L., & Pols, C. F. J. (2024). A hands-on activity to introduce the structure of NV-center quantum bits in diamond. *Physics Education*, *59*(4), Article 045017. https://doi.org/10.1088/1361-6552/ad4765

Physics Education

PAPER • **OPEN ACCESS**

A hands-on activity to introduce the structure of NV-center quantum bits in diamond

To cite this article: Rutger Ockhorst *et al* 2024 *Phys. Educ.* **59** 045017

OPEN ACCESS

PAPER

Phys. Educ. **59** (2024) 045017 (6pp)

iopscience.org/ped

A hands-on activity to introduce the structure of NV-center quantum bits in diamond

Rutger Ockhorst*, **Lodewijk Koopman and Freek Pols**

Science & Engineering Education, Delft University of Technology, Delft, The Netherlands

E-mail: r.ockhorst@tudelft.nl

Abstract

For the start of a secondary school level lesson series on quantum computing, we designed a hands-on modeling activity where students construct a model diamond lattice with a nitrogen vacancy (NV) defect. NV centers find application as qubits and sensitive magnetometers. This activity aims to help students visualize the structure of such NV centers within the diamond lattice, making the subject matter more tangible. The activity has proven to be challenging but feasible. It features both collaborative and competitive elements thereby surely creating an energizing buzz in the classroom.

Keywords: quantum computing, NV center, modeling

1. Introduction

Given its societal impact, e.g, in finance, medicine and policy making, it seems reasonable that *all* students familiarize themselves with the basic concepts of quantum computation and sensing [1, 2]. This assumption implies that the subject should be part of the secondary school science curriculum.

A variety of activities and lesson materials that introduce students in high school to quantum computing already exist, see, e.g. [3, 4]. Such materials usually focus on the mathematical and theoretical aspects of a two-level quantum system also known as a quantum bit (qubit), regardless of the physical realization of such a system. The benefit of such a general approach is that the computational rules of qubits can be applied to systems based on either solid-state physics, photonics, superconductivity, or similar technologies. However, to make quantum technology more tangible, especially to novices, we feel that it would be beneficial to explore the physical realizations of qubits.

* Author to whom any correspondence should be addressed.

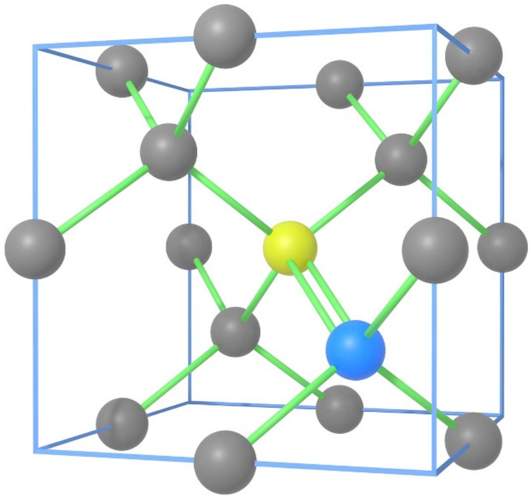

Figure 1. Schematic representation of a diamond lattice with a nitrogen (blue) vacancy (yellow) center substitution.

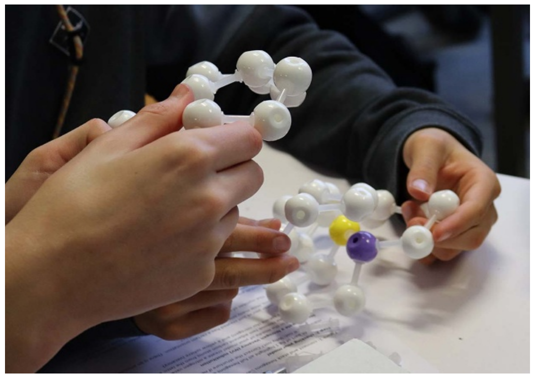

Figure 2. Using a chemical modeling kit to construct a diamond lattice with an NV substitution.

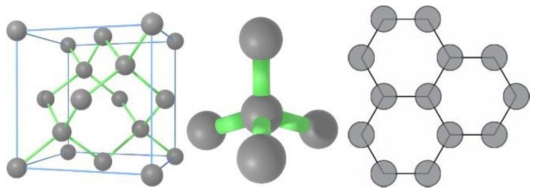

Figure 3. Some common depictions of the geometrical structures found in a diamond lattice: an FCC unit cell (left,) a tetrahedral structure (center) and a plane of hexagons (right).

As we are not aware of secondary school teaching materials that provide a consistent framework to study a specific physical implementation of a qubit, we took up the challenge of developing one.

A nitrogen vacancy (NV) center in diamond is one possible physical implementation of a qubit. The NV center consists of a nitrogen substitution with an adjacent vacant site in the diamond lattice, see figure 1. This results in five unbound electrons around the vacancy: one from each of the three adjacent carbon atoms and a group of two electrons in a *p*-orbital contributed by the nitrogen atom. When an additional electron is trapped at the vacancy, a charged NV^- center is formed. The six electrons in the NV^- center collectively act as a spin 1 system, which can be used as a qubit [5]. As NV centers in diamond play a prominent role in current quantum mechanics research and technologies, we may use it as one approach to introduce students to the ideas of qubits.

The activity described in this paper is part of an Erasmus+ project which aims to develop and test a lesson series on quantum computing for students at the secondary school level.

2. Activity design

To first familiarize students with the structure of diamond and the substitution of an NV center within the diamond lattice, we developed the following activity, which was inspired by [6].

Groups of two to four students are provided with 39 (white) spheres and 57 connecting rods as found in chemical modeling kits (figure 2).

Students are challenged to construct a model of a perfect diamond lattice. Clues on how to do this are provided in the form of common descriptions and pictorial representations of the diamond lattice, i.e. diamond having a tetrahedral structure, consisting of layers of hexagons and the face-centered cubic (FCC) structure of the unit cell (figure 3). Specifically, they are prompted to create a layer of three hexagons and stack three such layers on top of each other. Although formulating the assignment this way sets a clear goal, the link between the FCC structure, the hexagonal plane and the tetrahedral structure is not obvious. Thus, even though it may seem a straightforward task to some, there are still many decisions and some unexpected pitfalls that students need to deal with—as will be discussed later.

Once a group has successfully constructed their diamond model, the teacher asks them to create an NV center substitution. The group is provided with a blue sphere to represent the nitrogen atom. To represent the vacancy, we opted to use a yellow sphere (usually used to represent sulfur in organic chemistry kits). Alternatively, the site of the vacancy may be left empty, to produce a literal vacancy. Students are asked how many different orientations of the NV center are possible. Inspecting the spatial structure of their model they should conclude that there are four such orientations.

In addition to the collaborative nature of the activity we have added a competitive element by framing the next stage of the activity as a race to be the first to build a combined lattice consisting of four qubits. Specifically, once a group has produced a finished single qubit lattice, they receive the additional challenge to find other groups with different qubit orientations and combine their models until all four orientations are present in a single, combined crystal, see figure 4. The addition of this extra challenge requires groups to shift from intra to inter group discussions, adding to more dynamic classroom discussions amongst students.

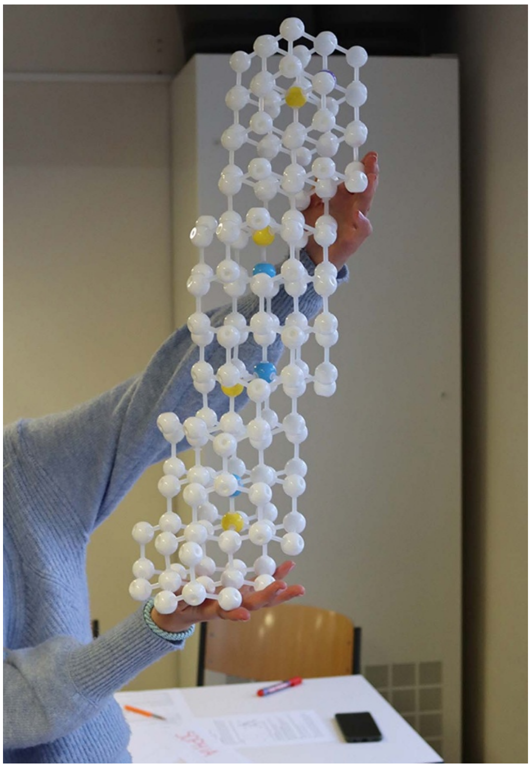

Figure 4. It is possible to build a model of four qubits using the materials provided.

3. Testing with teachers

The activity was initially tested with a small group featuring secondary school teachers ($N = 6$) and PhD Researchers ($N = 2$) from Austria, Denmark, and the Netherlands in November 2022. All participants were part of an Erasmus+ project to develop lesson materials on quantum computation. The activity was subsequently used by secondary school teachers in a one-week masterclass for 40 international students aged 16 and 17. The aim of this field test was to show that such lesson materials are suitable for secondary physics education.

3.1. Conducting the activity

In the teacher session, the strategies and dynamics employed to complete the assignment varied greatly. For instance, some groups dived in with all group members sticking carbon atoms together in a hap hazard way. Other groups put one person in charge of the main assembly process with other group members taking on an advisory role. We have also seen groups taking a more theoretical approach and first study the geometry of the lattice in more detail. This all happened unprompted and brought a great deal of enthusiastic buzz into the room.

It is likely that some students will be hesitant to start since it is all new to them, and the desired outcome is still unknown. Although this could be resolved through minor guidance from the teacher, we would propose not to abandon the discovery phase in favor of a more structured start, provided the teacher is willing to jump-start groups where necessary.

During this initial testing, we noticed that the FCC unit cell is of little use. This could have been anticipated by noticing that some of the carbon atoms in the unit cell seem to float within the cell because they do not share at least one connecting rod with another atom within the same cell. We therefore removed the FCC picture for future

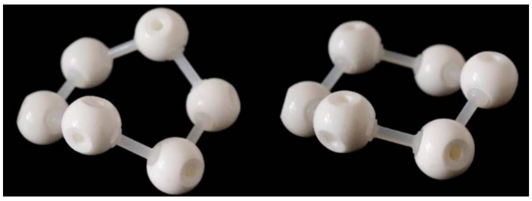

Figure 5. Boat (left) and chair (right) conformations.

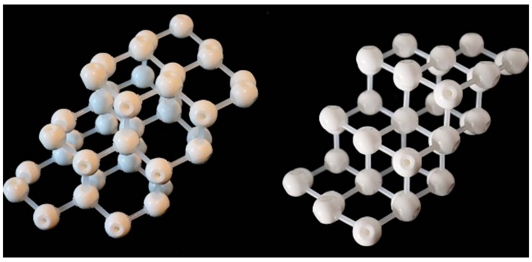

Figure 6. FCC diamond with ABC stacking.

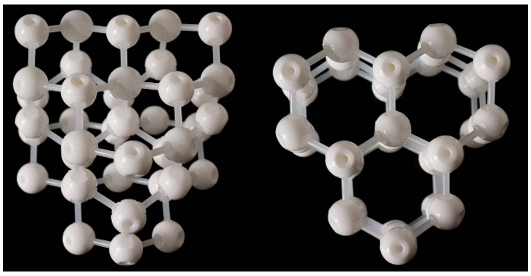

Figure 7. Hexagonal diamond with AB stacking.

iterations of the activity. We replaced it with a representation of tetrahedral geometry.

Groups quickly discovered that it is impossible to create a base layer of three hexagons that lies flat on the table: the spheres will zigzag up and down slightly. There are two possible zigzag patterns: either the so-called boat or chair conformations, see figure 5. Both conformations produce a viable lattice, but regular diamond contains only the chair conformation.

The relevance of the choice of a conformation presents itself when groups start stacking layers on top of each other: a layer of three hexagons in chair conformation will not stack neatly onto a layer in boat conformation. Moreover, to create the snowflake-like, staggered conformation between hexagon layers that is found in regular diamond structure, the layers must be shifted relative to each other producing a staggered ABC stacking pattern, see figure 6.

The model then displays a distinctive slanted face. Alternatively, layers can be stacked to produce a lattice that displays an eclipsed AB stacking pattern that 'grows' straight up. Even though this can be viewed as a different translation compared to the ABC stacking, in practice it often is the result of flipping the middle layer (in chair conformation) 180° along its long axis compared to the two outer layers. Viewing this structure from the side reveals several hexagons in chair conformation formed between layers. This is representative of a rare allotrope of carbon called lonsdaleite, see figure 7. Spotting either the staggered or eclipsed conformations proved to be an effective way to identify the correct crystal structure.

Issues such as conformation and stacking arrangements presented themselves naturally during the construction process. First getting participants started with the construction of their model lattice and discussing such details as they presented themselves, appeared to result in a natural flow of meaning making during the activity. (Unavoidably, some groups will stumble upon the correct solution right away. To encourage these groups to explore the subtleties of the diamond lattice, they can be paired with a group that has built a lattice that does not produce the diamond lattice and have them discuss the differences. By timing the disclosure of hints and information the teacher controls the progression of the activity.) We noted that teachers use different approaches to foster such discussions, depending on the sentiment of a specific group, from asking questions and giving subtle hints to full-fledged explanations.

During testing, we realized that there are still more allotropes of carbon which can be discovered. For instance, in both sessions we observed groups well underway constructing Buckminster fullerenes.

Overall, the race to produce a larger 4-qubit lattice took 45–60 min, depending on the length of teacher instruction and time allotted to the initial discovery phase.

3.2. Feedback from the teachers

The feedback provided by teachers after the trial session indicated that the activity is well suited to be incorporated in the lesson materials and that it matches well with the prior knowledge of their students. Originally, the activity was to be conducted on the third day of the masterclass. However, it was suggested to use this activity as an 'ice breaker' and introduction to the rest of the teaching and learning sequence on quantum computing. Thus, it was moved to the first day of the masterclass. Teachers reported that students were motivated to complete the activity. It also motivated students to study the lesson materials about quantum computing to which the activity was an introduction. Furthermore, the activity enhanced the social interaction between participating students from different countries.

3.3. Limitations and improvements

In discussing the activity with colleagues outside of the Erasmus+ project, some voiced the concern that the ball and stick models of chemistry may be enforcing a model of localized particles which may hinder students' development of notion like wave-particle duality or superposition that are often deemed crucial aspects of the quantum world. We agree that such issues can and should be addressed in the remainder of the teaching sequence, further detailing the physics of the NV center. At the same time, it is precisely because the diamond lattice is such a rigid structure at room temperature that we can study the quantum nature of the defect inside of it. Furthermore, it is the relative localization of the NV center that enables its use as a qubit and a nanoscale magnetometer. It is an opportunity for the teacher to address the uses and limitations of models, and we encourage them to take it.

We have identified a few ways to add some features that could further enhance the activity. Firstly, we have 3D printed several transparent spheres to represent the vacancy. This way, the idea of the site being vacant is conveyed more strongly than with the yellow sphere without sacrificing rigidity of the model.

Secondly, and in the same vein, the sphere representing nitrogen taken from an organic chemistry kit usually has the same shape as the carbon spheres with the same tetrahedral geometry and thus four connection sites. However, nitrogen has a covalence of three instead of four, with an electron pair in one of its p-orbitals. The electron pair could be represented by a custom 3D printed connecting rod or stub with two protrusions, one for each electron. When creating the NV substitution, students may then verify that there are five electrons involved in the NV center if the two-electron stub is added to the nitrogen atom. We have excluded a model for capturing the sixth electron in the vacancy to create the NV^- center. This is also to be addressed in the follow-up teaching and learning sequence.

4. Conclusion

In this article we presented an engaging activity that can be used in a broader teaching and learning sequence on quantum computation and quantum sensing, specifically on the physical implementation of a qubit or atomic magnetometer. We have found the activity to be challenging and engaging for both secondary school students and teachers in equal amounts. As a testament to this, one of the authors confesses that during the initial design of the activity he produced a lonsdaleite lattice instead of regular diamond and that it took about a week to figure out that there was more to the construction of a model diamond lattice than meets the eye.

Data availability statement

The data cannot be made publicly available upon publication because they are not available in a format that is sufficiently accessible or reusable by other researchers. The data that support the findings of this study are available upon reasonable request from the authors.

Acknowledgments

We acknowledge support from the Erasmus+ programme of the European Union and from the Dutch ministry of Economic Affairs and Climate Policy (EZK) through the Quantum Delta NL programme. We thank all students, teachers and scientists involved. We thank TU Delft's QuTech

Taminiau Lab for providing the chemistry modeling kits.

Ethical statement

This study has been approved by our institution's ethical commission, letter of approval 2635. Participating teachers were briefed on the purpose of this study and provided informed consent for the results to be published.

ORCID iD

Freek Pols https://orcid.org/0000-0002-4690-6460

Received 21 November 2023, in final form 17 April 2024
Accepted for publication 3 May 2024
https://doi.org/10.1088/1361-6552/ad4765

References

[1] Fox M F J, Zwickl B M and Lewandowski H J 2020 Preparing for the quantum revolution: what is the role of higher education *Phys. Rev. Phys. Educ. Res.* **16** 020131
[2] Aiello C D *et al* 2021 Achieving a quantum smart workforce *Quantum Sci. Technol.* **6** 030501
[3] Bondani M *et al* 2022 Introducing quantum technologies at secondary school level: challenges and potential impact of an online extracurricular course *Physics* **4** 1150–67
[4] Hughes C, Isaacson J, Perry A, Sun RF and Turner J 2021 *Quantum Computing for the Quantum Curious* (Springer)
[5] Childress L and Hanson R 2013 Diamond NV centers for quantum computing and quantum networks *MRS Bull.* **38** 134–8
[6] Delft University of Technology 2019 Researchers report MRI on the atomic scale (Phys.org) (available at: https://phys.org/news/2019-12-mri-atomic-scale.html) (Accessed 12 October 2023)