CrystalWeb

"Crystals you can play with!"

Interactive Crystallography Website
Project Proposal

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Abstract

The CrystalWeb website will serve as an educational tool for students learning about crystals and as a database resource for people seeking information about specific crystal structures. Since three-dimensional crystal structures are generally difficult to visualize in two-dimensional space, interactive applets allow users to manipulate crystals on the web. These applets will come from AtomicControl software designed for this project and distributed through the website as well. In addition, because few online databases provide user-friendly online resources for crystal structures, a user-friendly database will be created to compile information about crystals for research purposes. Ultimately, CrystalWeb will provide students and researchers the tools that they need in school and in research. The web interface makes these goals possible on a global scale while promoting interest in the fields of crystallography and materials science.

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1. Introduction

1.1. Background

Materials Science has become an increasingly important technological field as nanotechnology comes to the forefront. Much of this field requires understanding and manipulating the atomic structure of materials in order to create uniquely new properties. Many materials in everyday life, such as metals and ceramics, are crystalline. Crystallography, the branch of science that studies the formation and structure of crystals, often refers to the generation of images portraying how atomic arrangements within a material. In single crystals, the crystalline arrangements of atoms are easy to see macroscopically because the natural shapes of crystals reflect the atomic structure. In addition, crystalline defects often control the physical properties of materials. Understanding crystal structure is vitally important to understanding the phenomena that occur at the cutting-edge of technology as well as in every day life..

1.2. Motivation

In colleges and universities, students studying materials science and engineering must learn the basics of crystallography in their core chemistry courses. The basic crystal structures found in large, complex objects are often impossible to describe with words or through two-dimensional drawings because of their three-dimensional nature. Difficult to understand on paper, the properties of complex crystal structures become very clear with models that rotate in three-dimensional space. At the university level, professors may facilitate the learning of crystallography by providing students with various ways to explore crystal structures.

We propose to create a website to provide resources that will allow users to learn about crystals by designing ways to manipulate crystal structures virtually so that students may learn and discover the nuances regarding crystals on their own.

Along with the lack of educational resources for students studying crystallography, there are few places on the internet devoted to amassing the increasing amount of data that we have gained about various crystal structures. Poorly designed sites that contain this information create burdens on researchers who may simply want to browse current data. Therefore, as an additional feature of our website, we will create a user friendly, easily searchable database of crystals and their structure, composition, and other details.

1.3. Objectives

CrystalWeb, an interactive crystallography website, will provide web-accessible tools for students and educators that will allow them to explore one-, two-, and three-dimensional crystals and to understand their structures on both microscopic and macroscopic levels. Our website will allow users to rotate crystals and view their distinctive geometries within Java applets. The content of the website supplementing the three-dimensional crystal models will describe the formation of different crystals and provide examples of crystals found in the environment. This website will include a crystal database that will provide researchers with a valuable resource to catalogue their findings and to search for crystal data. To give students a means to enhance their understanding of crystal structures, CrystalWeb will be a portal for the distribution of AtomicControl, a shareware program that enables users to design and investigate their own crystals. The website will also contain detailed documentation and instructions for the crystal-building software.

1.4. Audience

The primary audience of this project is the population of students studying materials science. Other people that we want to reach are people who are interested in learning about crystallography on a basic level. We also want to reach researchers in the fields of materials science and crystallography by designing the user-friendly, comprehensive crystal database.

2. Project Description

2.1. Layout

The main divisions of pages within CrystalWeb will be the education section, the database, and the software download page. Along with the home page, these will form the start of the user's CrystalWeb experience. The home page will welcome visitors, discuss the purpose for our project, and display a random "Crystal of the Day" to pique the interest of those who may be unfamiliar with crystallography. The education section will contain crystal structures and their descriptions, information about diffraction and other ways to determine crystal structures, and the mathematics and geometries associated with the field of crystallography. We intend for the educational section to provide students with a brief overview of various topics in crystallography. The database

section aims to provide researchers with a powerful search tool to find the properties of known crystals. Finally, the software download page will contain links to AtomicControl, a shareware program available through CrystalWeb, as well as software documentation and an online manual for building crystals within the program. Figure 1 portrays the detailed site map layout.

Figure 1: CrystalWeb site map

2.2. Prototype Visual Design

The preliminary graphical design for the website will undergo many changes in the future. The aesthetic components of our website will adapt to our perceived needs in the future, but the following diagrams illustrate some of the ideas that we have for the layout of the final site. The preliminary design is very clean and minimalist. The graphical content of 3D animations does not require a busy site design. The navigation scheme attempts to be simple and transparent, allowing users to find things quickly even if they are unfamiliar with the site. Figure 1 portrays the general layout of the website, including the navigation system and example content for an educational page. An interactive 3D model of a face centered cubic lattice exists alongside text describing its characteristics.

Figure 2: Screenshot of preliminary site design.

2.3. Navigation

In order to navigate the high-level sections of this design there is a persistent navigation bar at the top of the page. This bar contains links to the "Home" page, the main "Education" page, the main "Database" page, and the "Software" page. It will also contain the project logo, which will also act as a link to the home page. Figure 3 contains the layout of the top navigation bar.

Figure 3: Top navigation bar

Since there are too many pages for complete navigation of the site to fit into the top bar, the secondary page links reside within the left side navigation bar. This bar will stay consistent for all pages within the heading (education, database, software) and will

indicate which secondary page is currently active. Figure 4 demonstrates the layout of the left side bar for the education section of the website.

Figure 4: Education side navigation bar

2.4. Technical Implementation

The website will run off an Apache web server on a Unix-based operating system. PHP Hypertext Preprocessor (PHP) will dynamically generate our web pages. By using PHP, separate pieces of the website, such as navigation and content, will combine on the fly, and dynamic content, such as database access, will integrate easily with the static components of the website. Cascading Style Sheets (CSS) will allow for more flexibility within design of the website. CSS permits the separation of content and design and helps to improve ADA compliance. Style sheets will define how the layout of content on the page, while the HTML content will only contain the text of the website and structural tags, such as headings, and lists. If the design changes in the future, it will be easy to change the style sheet, while keeping the HTML content the same.

2.4.1. Visualization Applets

The main innovation of CrystalWeb will be its ability to provide 3D models of crystals with which users can interact. To realize this objective in the website format, we will use Java applets. These applets will exist with the text of the website to add a physical view to the textual description. Utilizing the visualization part of the previously developed AtomicControl software, the applets will allow users to rotate crystals while they read about them in the accompanying text.

2.4.2. Database Implementation

A MySQL database will store and retrieve crystal data for the Crystal Database section of the website. PHP integrates well with the MySQL database and generates viewable HTML content from MySQL database queries. The database will store the crystal's name, description, and crystallographic information. PHP will retrieve crystal data and format it so that the visualization applet can display a 3D picture of the crystal. Figure 5 provides an example of how the MySQL database may be implemented with sample entries.

id	name	description	formula	bravaislattice	sgnum	atoms
1	diamond	Purrrrdy (fancy too)	C	NULL	NULL	NULL
2	graphite	Used in pencil 'lead' 3	C	1	NULL	NULL
3	table salt	like a cow might lick	NaCl	NULL	NULL	NULL
4	pzt	piezo electric makes	PZT	NULL	NULL	NULL
5	cheese	moooooo	Milk	NULL	NULL	NULL
12	Water	aqua!	H₂O	NULL	NULL	NULL
11	Sand	glass / sand	SiO₂	NULL	NULL	NULL
10	ed	test	E Dy	NULL	NULL	NULL

Figure 5: MySQL database table with sample "crystal" entries.

2.4.3. AtomicControl

This project originally began as the software development of a standalone crystallography application called AtomicControl. This program can generate user created crystals and provides a visualization module to view these crystals. The user interface will be easy and straightforward to use, using a point and click model for all operations. AtomicControl is currently incomplete, but it includes basic crystal building and visualization functionality. The program was written in Java using the Java3D API for 3D visualization and Swing for the 2D interface. Due to AtomicControl's modular design, the visualization part of this software embeds easily into a Java applet. Users will need to have Java installed with the Java3D extension, and the website will contain instructions and links on how to install this software for those who do not already have it. Figure 6 gives the user a feel for the AtomicControl interface as well as its graphical capabilities in modeling the atomic structure of crystals.

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Figure 6: AtomicControl Screenshot

3. Project Management

The nature of this project requires effective and timely communication among all team members. In order to achieve this goal, we will setup weekly meetings to update each member on the progress of the project and ensure coordinated understanding of each member's tasks and responsibilities. The responsibilities of the project will fall into four general components: website and graphics design, database design, site content, and documentation. However, the responsibilities of each member will include a variety of duties.

3.1. Member Roles

Brief profiles of each team member and their general duties follow below. Many of the responsibilities will be shared among team members to ensure the overall success of the project.

- Edward Barnard, a Material Science and Engineering major, will be involved in much of the website and database design for the crystal structure. Since he developed AtomicControl, he will be overseeing the technical aspect of embedding the crystal modeling applets into our website. He will also develop the skeleton site using PHP and is the most proficient coder of the group.
- Stephanie Silberstein, another Material Science and Engineering major, will be involved in website and graphics design. She will ensure that the completed website

is functional, easy to use, and aesthetically pleasing. Stephanie will also contribute to the site content because of her background in material science.

- Frederick Wang, an Electrical Engineering and Biology major, will be involved in the graphics design of the website and will assist Ed in the database design and implementation. He will also contribute to the documentation of the project.
- Harris Wang, a Physics and Math major, is the project manager and will oversee the progress of the project. He is in charge of ensuring that all members remain in good communication with one another. He will be assisting with the site content and database design as well as documentation of the project.

Since multiple members will work on the same site files, we will use subversioning software on an ftp server/client system. This will allow each member to upload their files onto a central server for all group members to view. Subversion will prevent versioning miscommunication and will ensure that all members are working on the most updated version of the site files.

3.2. Timeline

We have divided the project into the tasks and milestones as shown in figure 7.

Figure 7: Gantt chart of tasks and milestones

4. Future Developments

The success of this project will depend on the number of people who will take advantage of the three-dimensional visualization software provided with the website. The development of the database will require the trust of researchers and a willingness on their part to input the data from their experiments for the benefit of other scientists. This website may one day serve as a replacement for the introduction to materials science course taught at MIT if the material may be integrated seamlessly with the site design and purpose of CrystalWeb.

5. Conclusion

We will design and implement the CrystalWeb website, providing educational tools for students and researchers through the creation of a database and the utilization of three-dimensional crystal modeling software. By accomplishing these tasks, we want students to come to a better understanding of the crystallography that they learn and how it may be pertinent to their future.