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MaterialVis: Material visualization tool using direct volume and surface rendering techniques

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ABSTRACT

Visualization of the materials is an indispensable part of their structural analysis. We developed a visualization tool for amorphous as well as crystalline structures, called *MaterialVis*. Unlike the existing tools, *MaterialVis* represents material structures as a volume and a surface manifold, in addition to plain atomic coordinates. Both amorphous and crystalline structures exhibit topological features as well as various defects. *MaterialVis* provides a wide range of functionality to visualize such topological structures and crystal defects interactively. Direct volume rendering techniques are used to visualize the volumetric features of materials, such as crystal defects, which are responsible for the distinct fingerprints of a specific sample. In addition, the tool provides surface visualization to extract hidden topological features within the material. Together with the rich set of parameters and options to control the visualization, *MaterialVis* allows users to visualize various aspects of materials very efficiently as generated by modern analytical techniques such as the Atom Probe Tomography.

1. Introduction

Extracting the underlying atomic-level structure of natural as well as synthetic materials is vital for materials scientists, working in the fields such as electronics, chemistry, biology, and geology. However, as the topology and other important properties are buried under a vast number of atoms piled on top of one another, this inevitably conceals the targetted information. Without any doubt, the visualization of such embedded materials can help to understand what makes a certain sample unique in how it behaves. However, rudimentary visualization of atoms would fall short because it will not reveal any topological structure or crystalline defects.

In order to visualize the material topology, the data must be represented as a *surface manifold*, whereas, visualization of crystalline defects require extracting and quantifying defects and representing the data *volumetrically*. Current visualization tools lack such features, and hence, they are not very effective for visualizing the material topology and crystalline defects.

Material visualization tools require atomic coordinates of the materials as input. Acquisition of real-space atomic coordinates of a sample has been a major obstacle, until recently mainly restricted to the surfaces. One can call this period as the *dark ages* of material visualization. However, recent techniques, such as *Atom Probe Tomography* [1], can extract atomic coordinates much easier than before. This is also a very active research field, with the promise of many new advances in the near future. Accordingly, as the data acquisition phase for materials gets more efficient and accurate, the necessity for sophisticated material visualization tools becomes self-evident.

Our motivation on *MaterialVis* is to provide such a visualization tool that can reveal the underlying structure and various properties of materials through several rendering modes and visualization options. In this way, we intend to provide a good material analysis tool that will be useful in a wide range of related disciplines. *MaterialVis* supports visualization of both amorphous and crystalline structures. Amorphous structures only present the topological features while crystalline structures present both topological features and defects. The structure of a material can be best visualized using surface rendering methods. The underlying surfaces of the material should be extracted and visualized. On the other hand, defects such as the disposition of some atoms, vacancies or interstitial

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impurity atoms in the structure, cannot be visualized by simply drawing the atoms or rendering the surface of the crystal. These defects can be best visualized using *direct volume rendering* techniques. *MaterialVis* supports direct volume rendering and surface rendering, as well as combining them in the same visualization. It provides the functionality-driven visualization of the same structure with several techniques; thus it helps the user to analyze the material structure by combining the output of individual rendering modes.

We tested the tool with three real-world and seven synthetic datasets with various structural properties, sizes and defects. For instance, the sponge dataset [2] is a material produced from silicate, which has interesting nano-technological properties. Very recently, it has been experimentally shown that a silicon-rich oxide film can decay into a silicon nanowire network embedded in SiO_2 by spinodal decomposition during rapid thermal treatment [3], which has also been confirmed by accompanying kinetic Monte Carlo simulations [4]. The underlying goal in such a line of research is to achieve a nano-scale feature control and transfer it to inexpensive large-scale thin-film technology for silicon-based optoelectronics through growth kinetics. However, the direct imaging of such structures through transmission electron microscopy has not been satisfactory due to low contrast between Si and SiO_2 regions. We believe that it forms an ideal candidate for demonstrating the need for a direct volume imaging tool.

The organization of the paper is as follows. First, in Section 2 we discuss related works to address where our contribution lies within the context of existing tools and similar studies. In Section 3 we outline the general framework of *MaterialVis*, followed by two sections on the preprocessing and rendering steps. In these sections the main algorithms are presented in the form of pseudo-codes, leaving technical details to the accompanying Supplementary Materials document. Some of the capabilities of the tool are demonstrated in Section 6 using an embedded quantum dot data set. Even though our primary emphasis in *MaterialVis* is on functionality, but not the speed, nevertheless in Section 7 we provide performance benchmarks for a wide range of datasets. Finally, a brief conclusion is given.

2. Related work

There are many commercial and free crystal visualization tools. *CrystalMaker* [5], *Shape Software* [6], *XtalDraw* [7], *Vesta* [8], *Diamond* [9] and *Mercury* [10] are some examples. There are also some studies on the analysis of crystals that also provide some visualization functionality, such as the work of by Ushizima et al. [11]. These tools are essentially crystal analysis tools, which also provide some visualization functionality. Their visualization capabilities are not very advanced. They mostly offer just atom-ball models with some variations. Some of the tools support primitive surface rendering, which allows examining the crystal on the unit cell level. However, they are not sufficient to examine the underlying topology of a dataset.

There are also general visualization tools such as *AtomEye* [12], *VisIt* [13], and *XCrySDen* [14]. These tools provide sophisticated visualization capabilities but they lack the ability to create volumetric representations of materials, cannot use direct volumetric rendering techniques, and cannot quantify defects of crystal structures.

Iso-surface rendering techniques provide fast surface rendering of the volume data. They are especially useful when the surfaces are the regions of interest for the volumetric data. Doi and Koide [15] propose an efficient method for triangulating equi-valued surfaces by using tetrahedral cells based on the Marching Cubes algorithm [16].

MaterialVis is primarily based on direct volume rendering. There are mainly two types of volume data. The first type is the regular grid representation, which is widely used in medical imaging. Mostly texture-based techniques are used for the visualization of regular grids. Earlier approaches use sampling the volume along the view direction with parallel planes [17,18]. New graphics cards allow storing the volume data as 3D textures in the GPU. Ertl et al. [19,20] use a pre-integration mechanism to render the volume using 3D textures. Regular grid representation can be rendered efficiently, but the datasets using this representation are very large. The second type of data, unstructured grid representation, can be significantly compacted, so it can give much higher detail levels for the same size.

Visibility ordering is an important part of volume rendering algorithms. Cook et al. [21] and Kraus and Ertl [22] propose methods for performing visibility sorting efficiently. Shirley and Tuchman proposed a projected tetrahedra algorithm [23] for visibility sorting. Wylie et al. [24] later extend this algorithm to GPUs using vertex shaders.

Garrity [25] and Koyamada [26] use connectivity information to traverse the mesh efficiently. Weiler et al. [27] extend this approach to GPU. Callahan et al. propose a visibility ordering algorithm, *HAVS* [28], which performs an approximate sorting on the CPU and refines the sorting in the GPU. Silva et al. [29] present an extensive survey of volume rendering techniques.

3. General framework

Fig. 1 illustrates the framework of *MaterialVis* which has two main stages: *preprocessing* and *rendering*. The preprocessing stage takes the raw input and constructs the volumetric representation. For (poly)crystalline structures the preprocessing step further continues and assigns error values to atoms representing crystal defects. The rendering stage visualizes the constructed volume representation. The input reader module reads the volumetric representation and initializes the renderers. At any time, one of five renderers is selected by the user and the visualization is performed. These renderers use the OpenGL-based drawing module to display the volumetric data. The rendering tool is an interactive tool. The user interactively provides various inputs to renderers, such as camera and light information and several renderer-specific parameters.

4. Preprocessing

MaterialVis operates on a very simple input format. For amorphous materials, the types and atomic coordinates of each atom in the material is sufficient. However, for crystalline structures, the tool also requires primitive and basis vector information of the crystal structure. If this information is not readily available, our earlier work, *BilKristal* [30,31], could be utilized to extract the unit cell information from the crystal structure.

MaterialVis construct a volumetric representation using the coordinates of a set of points representing atoms in the material. There are two types of volumetric representations: *regular* and *unstructured* grids. Regular grid representation is widely used in medical imaging fields where the input data is fixed in resolution. For material visualization, interest points are the atoms; crystalline defects are attributed to them and they constitute the surface structure. Because the regular grid representation is defined independent to atoms, a fairly high grid resolution must be used in order to capture crystal defects and surface structures in high detail. On the other hand, unstructured grid representation uses atoms as vertices. Accordingly, despite using the connectivity information, the unstructured grid representation is more compact and suited