AURAL STRUCTURES: MUSIC AS A TOOL TO DESCRIBE CRYSTALS AND THEIR ORIGIN

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Abstract

Aural Structures is a project aimed at producing musical models of crystals for educational applications. Traditionally, music has been used in STEM teaching to help memorising scientific concepts. However, music (without lyrics) can also be considered in itself as an interesting way to explore and explain the complexity of both natural and artificial structures, guiding learners of any age towards the deep understanding of the concept of molecular order. Our model of crystal structures was used to give an aural representation of crystals to improve memorisation and learning through emotional involvement. All sound parameters (pitch, duration, timbre, and dynamics) are based on physical, chemical and structural properties of the atoms involved in the crystal. Possible applications of this novel educational approach will be illustrated with practical examples about some relevant topics of mineralogy (e.g. solid solutions, polymorphism). We are currently designing a software that, given the chemical composition and the space group of a given crystal, automatically carries out our approach to generate its musical model. Starting from a file describing the crystal's chemical features in standard format, it will extract the crystal structure parameters and scan the structure in order to obtain the musical score and play it. Such a software might be extended to change the sound rendering of the structures based on additional parameters, in order to fit different educational purposes. In parallel with the development of the software, we are currently exploring the possibility of using aural models as a blueprint for producing original musical compositions. We performed such compositions with a 12-element orchestra in front of an audience of high school students (K10-12), within a format including seminars and a final concert. Musical conduction directly involved the students in the performance, namely in the sonification of crystallization/fusion/vitrification processes. Music, in association with pictures and short movies shown during the musical performance, proved an interesting way to explore and explain the complexity of natural processes for understanding the concept of molecular order/disorder.

Keywords: Music, Mineralogy, Crystals, Sonification.

1 INTRODUCTION

As a scientific discipline, crystallography has contributed many ground-breaking achievements in elucidating the structure of matter at or near the atomic level of detail, from the simplest inorganic salts to functional complexes or proteins, resulting in 29 Nobel Prizes [1 and references therein]. As a consequence of its highly interdisciplinary nature, crystallography is universally known as a powerful scientific tool in STEM (science, technology, engineering, mathematics) studies as well as a vehicle for investigating the structural and technological properties of the materials. From the first experiments of Laue and Bragg [2], graphical representations and solid models of crystal structures have been widely used to illustrate the features of the complex atomic arrangements in crystalline materials.

Today, crystallography teaching routinely employs visualization software including Diamond and Mercury [3,4] to allow the study of the crystal structures also in terms of symmetry content. These software, also used in research activities, make possible the investigation of the crystal structure along any crystallographic direction, allowing the identification of the symmetric axes operating in the crystal and the study of related structural properties.

In addition, crystallographic databases (i. e. Cambridge Structural Database [5,6], https://mindat.org/) provide new opportunities of teaching crystallography. For example, the Crystallography Open Database [7,8] and Protein Data Bank [9] are used in University courses to provide examples of case studies [1].

Recently, with the advent of inexpensive 3D-printers, three-dimensional printed crystallographic models are widely used in classes and museum activities [10,11].

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However, all above-mentioned teaching supports are based on visual perception. Such approach for very complex structures sometimes is not sufficient to fully understand structural atomic arrangements. Therefore, the addition of a second aural perceptive channel can be a valid support to the learning process. In Monno et al. [12] we introduced a method of sonification of crystal structures to provide such support. The present work presents the state of the art of the aural modelling of crystals and provides some examples of educational application. Finally, a discussion of the obtained results and future perspectives is reported.

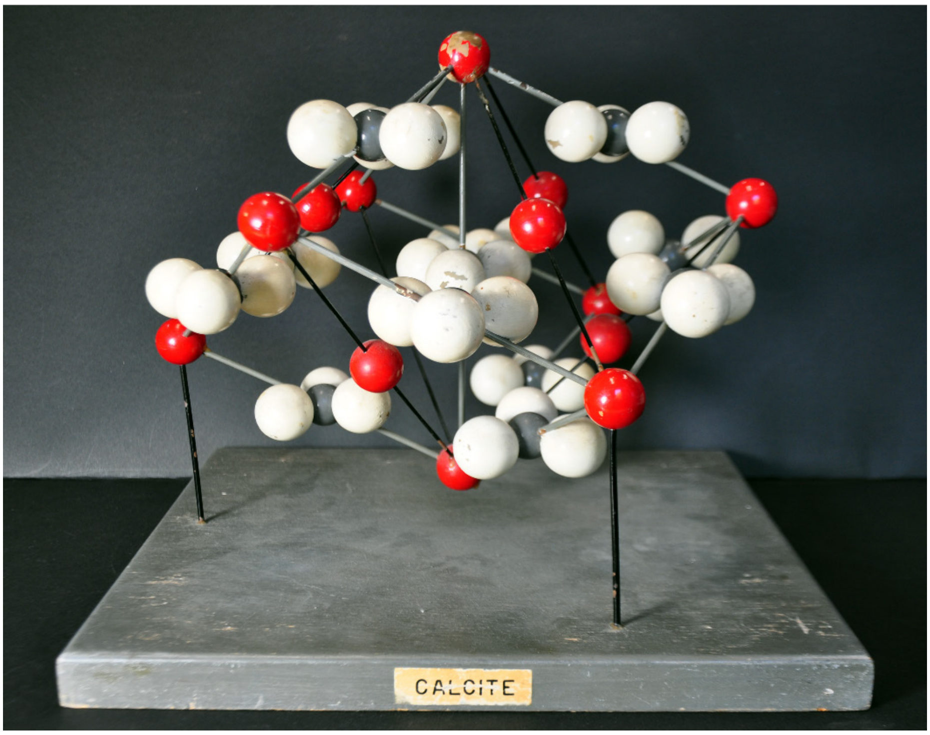

Figure 1. Wooden model of calcite with rhombohedral unit cell.

2 PERCEPTION AND SONIFICATION

The mental processes involved in the higher-functions of the brain (e.g. perceive, thinking, memorization, planning, etc.) can be gathered in the term *cognition* [13]. A key role in cognition is played by *perception,* a set of processes whereby we make sense of sensory impressions created by the detection of environmental stimuli. It should be considered that the perception is a complex interactive process where the sensory inputs (bottom-up process) are combined with the existing concepts and memory (top-down). In the sequence that constitutes the processing of information (transformation, reduction, elaboration, storage, recover, and use of the sensory input) each one of the five senses involves different neural networks and different consequences [14]. To stay on the subject of this paper, the visual and auditory perceptions are mainly related to the display of crystal structure and composition. The visual perception of the crystal structures through simplified solid or graphic models (e.g. Krantz models, molecular models) were and still are the main educational supports in mineralogy and crystallography. Indeed, they are idealized and analogical models of crystal unit cells, where atoms are represented by spheres of different size with characteristic spatial distribution (Fig. 1). Aural perception, like the visual one, allows spatial resolution to locate in space a given stimulus and thus may offer an effective way to translate in the auditory display the structure and composition of crystals. The added value of an auditory display of the crystal structure and composition resides in the involvements of neural regions of the primitive brain structures dealing with motivation, reward, and emotion [14,15]. Furthermore, if on one hand this multiplies the possible significant relations to decode and learn, on the other hand it provides a more effective emotional involvement to ease memorization.

In the last decades, the birth and rise of sonification [16] as a multipurpose tool able to give an auditory rendition of data of different nature, provided a theoretical and practical framework to obtain auditory displays for scientific, educational and industrial scopes. Sonification is considered a subset of functional sounds and several strategies are possible [16]. The Parameter-Mapping Sonification (MBS) and symbolic sonification are here used to give an aural model of crystals and crystallisation process, respectively.

3 METHODOLOGY

The details of the method used for sonification have been described previously [12]. Basically, the modelling of crystal phases was obtained through the scanning of the atom positions occurring in the unit cell on virtual planes perpendicular to a specific direction, conventionally aligned to the main symmetry axis of the structure. The sonification strategy provided for the conversion of four crystal parameters: the chemical 1) group(s) and 2) period(s) of each atom and the 3) angular and 4) Euclidean distance determined by scanning axis (i.e. polar coordinates) in the unit cell, into four sound parameters: 1) duration(s); 2) timbre(s); 3) pitches; 4) dynamics.

The first step to take is to define the *operative cell* for each crystal phase according to its crystal system. In the case of calcite, two possibilities occur: a trigonal unit cell (rhombohedral) or a hexagonal super cell (x4). This double possibility is only present for the crystals of hexagonal/trigonal system. Once identified the symmetry axes of the crystal, they became the scanning directions of the sonification. The complete aural model of a crystal consists of the scanning of the characterizing symmetry axis, followed by the ones of the secondary symmetry axes.

The definition of the parameters for sonification was the first step to write a code to transform a given crystal phase in a musical model. The overall procedure for obtaining our output can be split into three main steps, as follows:

1 Pre-processing. Starting from a standard file reporting the chemical data about the crystal, the spatial representation of the unit cell is obtained, where each atom is associated with its Cartesian position in the 3D space and with its element.

2 Structure reading. For each symmetry axis associated to the crystal's structure, which will provide a portion of the final score, a scanning direction is determined, and using polar coordinates the cell is scanned along this direction by a virtual plane; whenever the plane meets atoms, the plane is scanned by virtual angles from 0° to 360°, generating notes as long as atoms are encountered and recording their timbre, pitch and dynamics based on their chemical and structural features.

3 Translation. The generated representation is converted into a music score or directly into sound, depending on the specific needs. Several output formats are provided for.

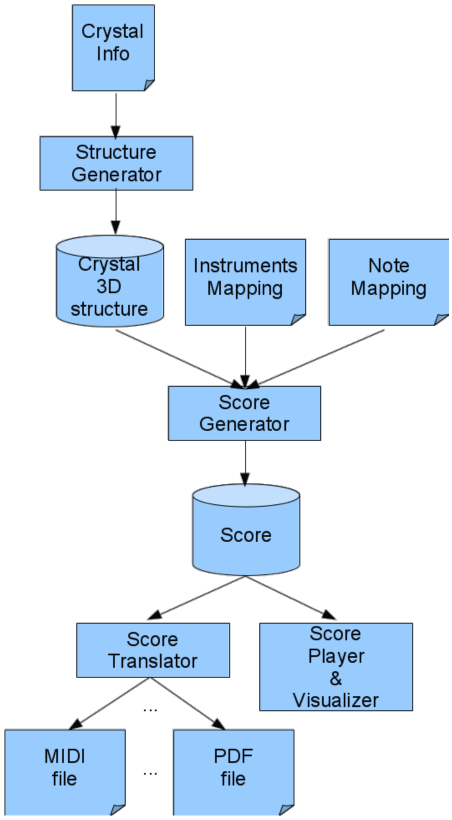

Figure 2. Schematic flow chart for the realisation of the sonification software.

The art of conducting with hand-gestures the musical performances (chironomy) dates back to Ancient Egypt [17]. Such practice is still present in modern conducting, thanks to the development of several musicians (e.g. Walter Thompson, Lawrence "Butch" Morris, Frank Zappa, John Zorn). This instant composing technique was used to involve the student audience and the Earth Ensemble of Uniba (composed of professors, students and technicians of our department) in a symbolic sonification of the crystallisation process. A body-gesture code was defined in order to musically perform crystal nucleation an growth, development of crystal defects, fusion and vitrification. Table 1 shows the sonification strategy to associate the state of the matter with the musical parameters.

Table 1. *Sonification strategy to associate the state of matter with the musical parameters.*

Musical parameters	**Solid**		**Fluid**	
	crystal	***glass***	***liquid***	***gas***
Time	striated	striated	smooth	smooth
Space	striated	striated-smooth	smooth-striated	smooth
Dynamics	*pp*	*p-mp*	*mf-f*	*ff*

4 EXPLAINING POLYMORPHISM WITH MUSIC

An example of educational use of crystal sonification is polymorphism, where two or more crystal phases share the same chemical formula (i.e. stoichiometry), but are distinguishable for symmetry (i.e. space group). A typical example of polymorphism is the one of calcite and aragonite. Although they have the same chemical formula ($CaCO_3$), they are characterized by very different symmetry (Fig. 3).

Calcite: space group: R -3c

Aragonite: space group: Pcmn

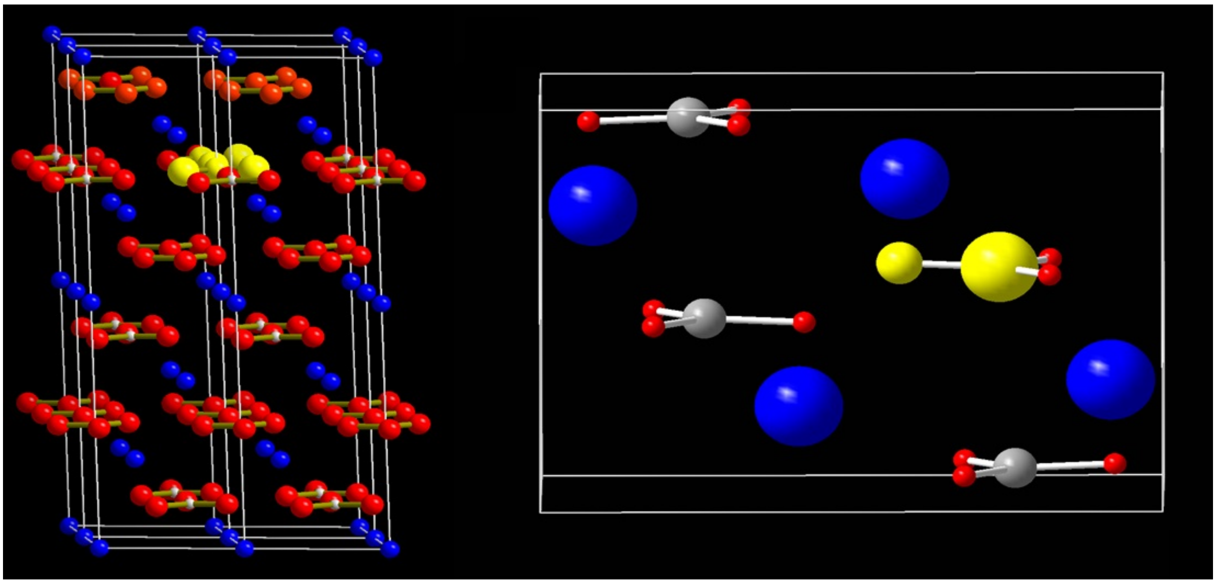

Figure 3. Operative cells for sonification used for calcite (left) and aragonite (right). Colour key: blue = calcium; grey = carbon; red = oxygen. In the combined visualisation of the auditory model, the scanned atoms are highlighted in yellow.

5 MUSIC CONDUCTION TO EXPLAIN CRYSTALLIZATION

In the last two years, our method of crystal sonification for teaching purposes has been presented to an audience on several occasions. In such occasions, we used a format based on short lectures, followed by a multimedia musical performance. The audience ranged from high school students, to established scientists of the National Institute of Geology and Volcanology. An overview of the activities related to the Aural Structure project is available on the dedicated webpage of the department (Fig. 4). A recent online article of National Geographic Italia [18] reports some information about the project.

Figure 4. QR-code to access the webpage of Aural Structures.

Figure 5. Personalised t-shirts for the components of the Earth Ensemble of Uniba according to the instrument/voice played.

The musical performance addressed specific phenomena, including crystal polymorphism, crystal growth, vitrification and crystal formation from magma. An orchestra of up to 14 “chemical elements”, each associated to a different musical instrument (Fig. 5) plays live-conducted improvisation based on the sonification strategy shown Table 1. The audience is involved in the musical performance after a short introduction to the body-gesture code (Fig. 6). The feedback from audience is enthusiastic and drives us to improve further this kind of educational experience.

Figure 6. Music conduction to explain the crystallisation process involving the audience and the Earth Ensemble of Uniba (see text for details).

6 DISCUSSION AND CONCLUSIONS

In a previous paper we presented a model of sonification aimed at providing aural translations of crystal structures [12]. Since then, we have used this method to develop learning activities, which in turn provided useful information for further implementation. The algorithm currently under definition (see Methods above) will allow us to establish new directions in our research. A specific software will be developed to "translate" 3D structures into music (and possibly the other way around, in an attempt to translate music into solid shapes). The program will be interfaced to holographic projectors for the full perception of crystal structures. Automated scanning of crystal structures (according to different atom features) on plans perpendicular to the symmetry axes will highlight the position of atoms and make them audible by associating them to given sounds. The software will allow the automated import of cell parameters of the crystal, as reported by current databases (mindat.org), extrapolating its "sound" according to the different directions of the symmetry axes in the minerals. It is therefore conceivable, that this approach will yield a huge number of musical models. Taking into consideration only mineral species, 4300 melodies can potentially be obtained by investigating just one axis. In addition, the musical heritage we obtain from natural items can be used as an inspirational source for composers and musicians. Musical compositions based on the aural translation of crystal structures have already been performed in our seminars/concerts. More opportunities of developing this creative aspect of our work is currently under definition within a collaboration with established composers. Our research also aims at developing exhibits for museums and science centres, in which the visitors will be encouraged to interactively explore crystal structures and the processes related to their formation. Multisensory perception will allow better understanding of the complex structural architectures of solid state crystals.

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