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THE GRAMMAR OF CRYSTALLOGRAPHIC EXPRESSION

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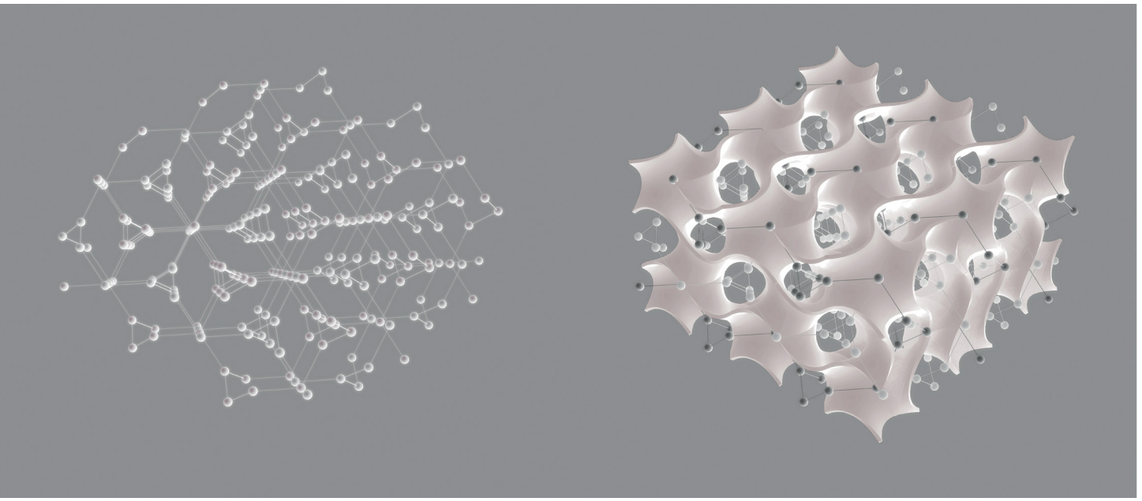

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ABSTRACT

This paper stems from a research collaboration which brings together two disciplines at different ends of the scale spectrum: crystallography and architecture. The science of crystallography demonstrates that the properties of crystalline materials are a function of atomic/molecular interactions and arrangements at the atomic level—i.e., functions of the form and structure of the material. Some of these nano-geometries are frameworks with special characteristics, such as uni-directional porosity, multi-directional porosity, and varied combinations of flexibility and strength. This paper posits that the symmetry operations implicit in these materials can be regarded as a spatial grammar in the design of objects, spaces, and environments. The aim is to allow designers and architects to access the wealth of structural information that is now accumulated in crystallographic databases as well as the spatial symmetry logics utilized in crystallography to describe molecular arrangements. To enable this process, a bespoke software application has been developed as a tool-path to allow for interoperability between crystallographic datasets and CAD-based modelling systems. The application embeds the descriptive logic and generative principles of crystallographic symmetry. Using this software, the project, *inter alia*, produces results related to a class of geometrical surfaces called *Triply Periodic Minimal* (TPM) surfaces. In addition to digital iterations, a physical prototype of one such surface called the *gyroid* was constructed to test potential applications in design. The paper describes the development of these results and the conclusions derived from the first stage of user testing.

1 The interwoven *srs* nets and the *gyroid* surface dividing these nets

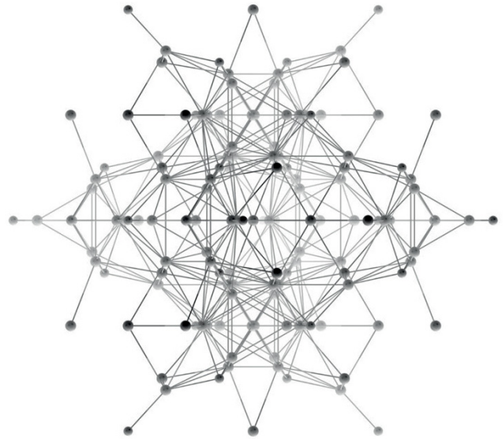
CRYSTALLOGRAPHICALLY INSPIRED ARCHITECTURE: A NEW PATHWAY FROM NANOGEOMETRY TO DESIGN

This paper has emerged from an ongoing collaboration between architects and crystallographers as part of a 30-month research project funded by the Leverhulme Trust in the UK. We formulated the project with the idea that creative practice, spatial practice, and design can be enhanced through their affiliation with fundamental science.

A handful of architects have published work related to symmetry concepts that resemble or are similar to crystallographic space groups. For instance, architects such as James Strutt and Gulzar Haider investigated complex symmetries and space packing concepts in the 1970s and 1980s. We value this previous work, but we think that our current collaboration goes much further. To our understanding, our project is the first long-term collaboration between crystallographers and architects that proposes instrumental and design outputs.

One goal of the project is for designers and architects to learn from the structure of matter at the atomic and molecular level, recognizing that structural features and symmetry operations found at nanoscales offer possible design diagrams with multi-scale potential. Thus, the project exposes designers and architects to the spatial symmetries utilized in science to understand the structure of matter at molecular scales. Until now, the full extent of the grammar of crystallographic expression has been beyond the disciplinary horizon of the design community worldwide. In advancing our interdisciplinary project, we believe that a full understanding of this grammar—along with tools to operate within the principles of spatial symmetry—will be highly advantageous to designers.

In order to develop this new kind of tool for designers, the project employs the principles of Rapid Application Development (RAD). RAD is an approach based on creating a functioning (bespoke) script as early as possible, and refining the result through feedback and iteration. The feedback comes from the eventual users of the system, and is used to refine the result in successive stages. At the present stage of the project, we have developed version 1.0 of the software application. In this paper, we report on the development of this RAD methodology



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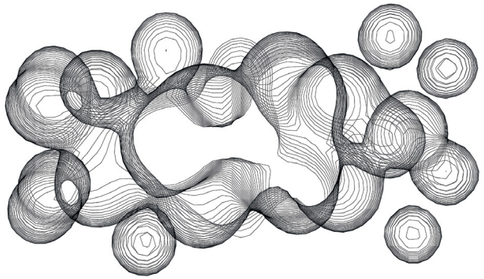

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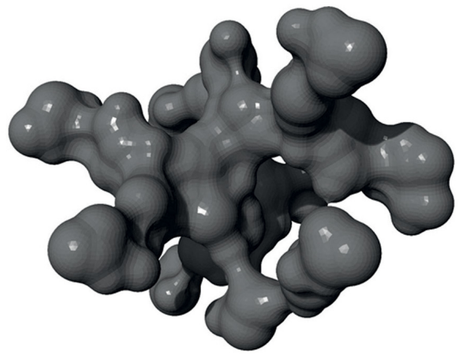

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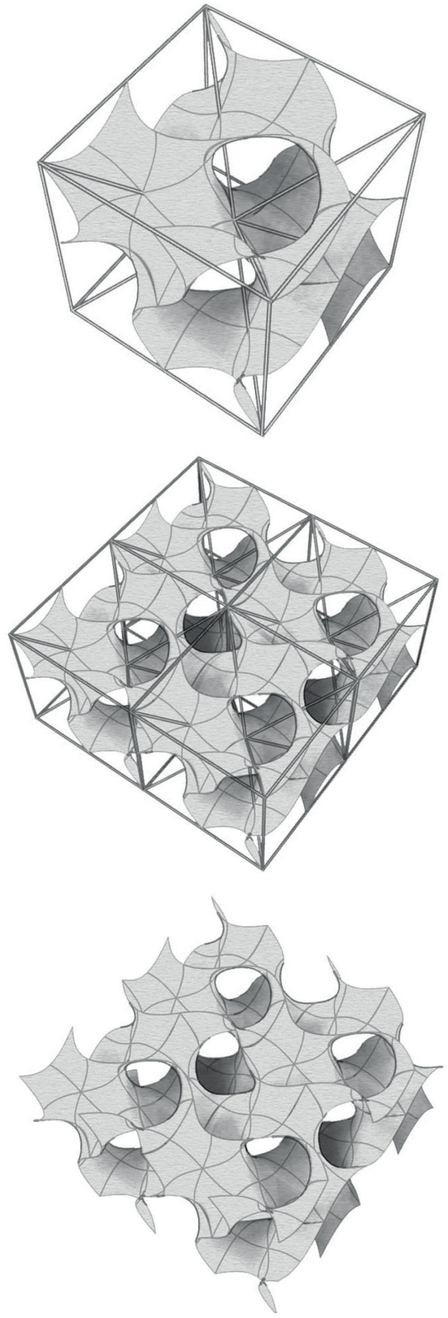
2 Expressive possibilities within the bespoke software application, based on a topology of points

3 Expressive possibilities within the bespoke software application, based on a topology of lines

4 Expressive possibilities within the bespoke software application, based on a topology of surfaces



5 The *gyroid* and its unit cell translated into a lattice

and how it was used in the production of a spatial/structural prototype. In April of 2016, we tested the application with our first user-group at the Smartgeometry conference in Gothenburg. The user-group comprised architects and architectural students.

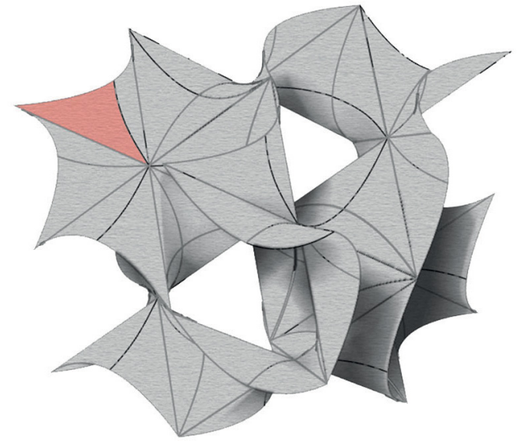
ENCODING THE CRYSTALLOGRAPHIC SPACE GROUPS

In the 20th century, the science of crystallography developed powerful procedures to analyze experimental data (specifically, X-ray diffraction data) in order to elucidate the structural properties of crystalline materials, which are based on two fundamental mathematical principles: periodicity and symmetry.

A crystalline substance exhibits three-dimensional periodicity. In other words, crystals have a high degree of repeat organisation in their structure, such that atoms, molecules, or ions typically repeat in regular arrays to form three-dimensional lattices with long-range order. The smallest repeating unit, which gives the complete periodic structure when translated in three dimensions, is called the unit cell. Further, the unit cell is an imaginary volumetric entity in Cartesian space, which defines within itself the positions of constituent atoms. These atomic positions are often related by symmetry, with symmetry operations that include reflection, rotation, inversion, and combinations of translation/reflection and translation/rotation. There is a finite number of combinations of these symmetry operations which can produce three-dimensionally periodic structures. Each such combination of symmetry operations is called a space group. Mathematics dictates that there are only 230 unique, three-dimensional space groups.

Within our project, we developed a design tool that allows designers to operate directly with any of these 230 space groups. The software application employs the principles of periodicity and symmetry to devise a generative process that simulates the assembly of molecules in crystal structures. It begins by selecting and importing an asymmetric unit from a crystallographic database, then runs through a series of operations to produce a periodic crystal structure. Thus, the interface allows for interoperability between existing crystallographic datasets and vectorial modelling systems in such a way that designers are able to not only simulate but also manipulate the crystalline assembly processes. *Rhino*, as one of the most widely used NURBS based CAD platforms, serves as the host environment and *Grasshopper* serves as its associated visual programming software. Within *Grasshopper*, the bespoke plugin application is programmed with *IronPython*.

Once the fundamental data has been simulated in *Rhino*, the application allows for designers and architects to give new



6 Construction of the *gyroid* based on the symmetry operations of space group 230

readings to these geometries by generating a range of expressive possibilities. In crystallography, various aspects of a crystal structure are understood through visualization techniques, which give rise to notable expressive potential. The application embeds the descriptive logic of crystal structures to create a language of form based on points, lines, and surfaces (Figures 2–4).

TRIPLY PERIODIC MINIMAL SURFACES

The idea of crystallographic space groups can be used as a tool not just to generate the "node and network" topology of crystal structures, but also to generate a class of surfaces called *triply periodic minimal* surfaces (TPM). In these surfaces, which exhibit periodicity in three dimensions, the asymmetric patch is a minimal surface stretched between a framework. The resulting surface is continuous and without breaks. One possible TPM surface is known as the *gyroid* (or the G-surface), which can be constructed by applying the symmetry operations of space group *Ia-3d* (space group number 230) onto a specific triangular surface patch (Figures 5 and 6).

TPM surfaces are of interest in science from several perspectives. On the one hand, TPM surfaces help visualize the more abstract properties of crystal structures. The *gyroid* reveals intriguing topological qualities by partitioning space into regular non-intersecting labyrinthine channels, with interesting optical abilities. The axes of these channels correspond to the vertices of two interwoven *srs* nets. In crystallography, a net or periodic graph is a mathematical abstraction which describes the topological framework of a family of actual molecular networks. One such class of nets is called the *srs* net, in which the vertices are three-coordinated figures. The *srs* net elegantly inter-threads with its enantiomorph in such a way that the structure is chiral—whereas one net is left handed, the other net is right handed (Hyde, O'Keeffe, and Proserpio 2008). The *gyroid* divides this pair of nets, mapping an equipotential surface between the two nets (Figure 1).

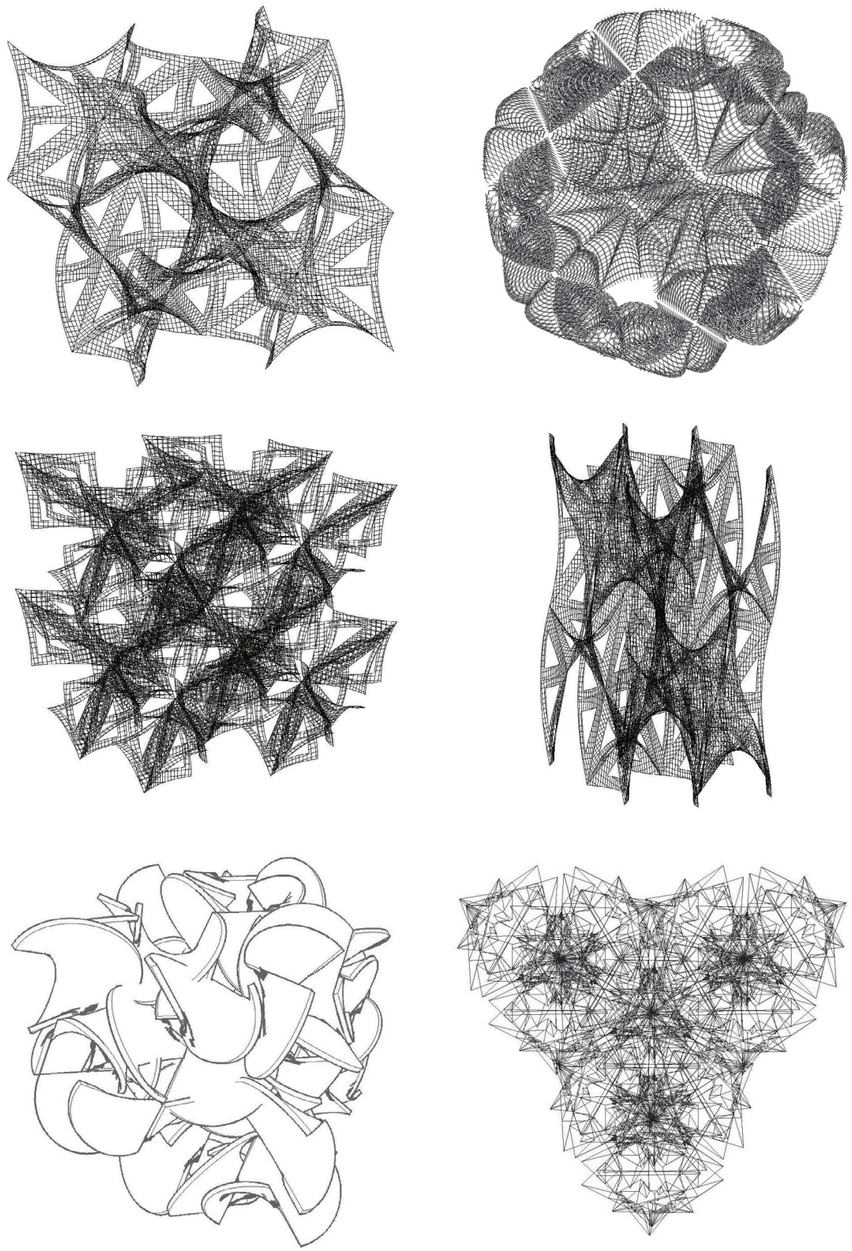
Furthermore, the extensive occurrence of TPM surfaces in nature indicates potential applications for their material properties. The *gyroid*, for instance, is now known to underlie the structural characteristics of many different types of material, from lipids in cells to synthetic polymeric molecular melts.

The construction of these surfaces has been known to crystallographers and mathematicians for many years, but the intricacy of their construction has not been widely discussed among designers. Furthermore, in the past, designers have not had access to tools that allow them to explore and utilize the symmetry operations of the crystallographic space groups. Our project aims to help designers and architects expand their understanding of space, structure, and form through these crystallographic processes.

The software application that we have developed was shared with a group of designers during the Smartgeometry conference in Gothenburg in April 2016, within a cluster entitled *Nano-Gyroids*. The workshop focused on learning to use the new software application, understanding how to utilise crystallographic space groups, and constructing *gyroid* and *gyroid*-like geometries. The workflow involved deriving new asymmetric unit patches, often with an affinity to existing molecular structures, and exploring the idea of symmetry inherent in the crystallographic space groups to build TPM constructs or alternative formations derived from the application of crystallographic symmetries. By varying the parameters of the seed patch and generating periodic structures using different space groups, participants produced a broad spectrum of digital iterations (Figure 7).

PROTOTYPE

After developing an understanding of their use in crystallography, participants of the cluster investigated ways of creating aggregates and morphologies inspired by *gyroid* formations and helped to develop a methodology to construct physical prototypes of the same geometry through alternatives to 3D printing. The resulting prototype—a lightweight structure assembled with prefabricated stainless steel members and fabric components—occupied 9 m^3 of space (Figures 8 and 9).



7 Wireframe views of constructs developed by workshop participants utilizing different space group symmetries

8 Initial prototype for the construction of a light-weight *gyroid* structure

The design of the lightweight structural system was partly inspired by the work of artist Alison Grace Martin, who has developed lightweight structures to build objects of mathematical interest. Before the workshop, she shared her structural ideas with the workshop leaders, inspiring us to develop a structural interpretation of *gyroid* and *gyroid*-like formations. This concept was further advanced with workshop participants, who developed morphologies for the final installation and helped to construct it.

CONCLUSION

The tools developed in our project so far have undergone a first round of testing by potential users. The users came from a broad spectrum of backgrounds in practice and academia. The results of the workshop suggest merit in our software, particularly as it systematizes the understanding of form and structure in its fundamental relation to material properties, and further provides a powerful interface for designers. In other words, the bespoke software is highly effective in allowing designers to operate with the grammar of crystallographic expression within a very short time frame.

In future, we believe that there are several significant areas in which the work described here could be developed and implemented. This new design work could operate at the crystallographic scale, at the architectural scale, or both. If regarded as a "blueprint" for designing objects, spaces, and environments, crystallographic geometries are highly significant, with applications such as:

- *Optical modulation:* crystalline structures frequently display properties such as uni-directional porosity, so that the material may appear opaque from most directions of view, but transparent when viewed in a specific direction. Components displaying these optical properties would be highly significant in modulating the levels of privacy of spaces, and their visual relationships to their surroundings.
- *Micro-climatic modulation:* the mono- and multi-directional porosity of crystalline structures sets them out as models with ideal geometries to regulate the enclosure and exposure of spaces with regard to an environment. Light, wind, water, and other environmental phenomena may be regulated through components with these geometrical characteristics.
- *Structural implementations:* among crystalline materials are structures with characteristics associated with strength or flexibility or both.
- *Sensing and actuation:* the combination of material assemblies that respond differently to changes in temperature allows for controlled use of the energy absorbed when they are exposed to sources of energy such as solar radiation. In such instances, sensing and actuation may be carried out directly through the interaction of these assemblies.

9 Prototype of a *gyroid* morphology as part of the *Nano-Gyroids* cluster at Smartgeometry 2016

9

ACKNOWLEDGEMENTS

1. We are thankful to the Leverhulme Trust for their generous support in making this research project possible.

2. We are thankful to Alison Grace Martin for sharing with us her knowledge in constructing iterative geometries. Our process in constructing a prototype of the *gyroid* was inspired by her work in constructing objects of mathematical interest.

3. We thank Smartgeometry 2016 and the participants in the *Nano-Gyroids* cluster who were integral in developing part of the work presented here: Pinar Aksoy, Marie Bartz, Giselle Bouron, Niklas Nordstrom, Marta Pakowska, Mauricio Rodriguez, Sebastian Andersson, and Liv Andersson.

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IMAGE CREDITS

Figure 1: Mallika Arora and Sergio Pineda, 2015

Figure 2: Sergio Pineda, 2013

Figures 3, 5: Mallika Arora, 2015

Figure 4: P. Andrew Williams and Mallika Arora, 2015

Figure 6: Mallika Arora, 2016

Figure 7: Clockwise from top left: Sebastian Andersson, Niklas Nordstrom, Marta Pakowska, Marie Bartz, Sebastian Andersson, Sebastian Andersson, 2016

Figure 8: Sergio Pineda, 2016

Figure 9: Daniel Davis, 2016

Sergio Pineda is an architect with experience in design research at the convergence of computation, fabrication, material science and emergent tectonics. After obtaining his Diploma from the Architectural Association in 2004, he worked for five years with practices in London (Foster + Partners, Adjaye Associates and Leit-werk) on a variety of award winning commissions in Barcelona, Denver, New York and Milan. He is currently based at Cardiff University, with a focus on collaboration between creative practice and fundamental science. In the past, he has collaborated with choreographers, sociologists, and hydrologists on initiatives such as the Architectural Association Visiting School in Medellin entitled Hydromeme.

Mallika Arora is an architect and computational designer with professional experience in Europe and Asia. She graduated with an MSc in digitally driven architecture from the TU Delft, and a B.Arch. from New Delhi. Mallika is interested in exploring the potential of computational design through a performative, methodological, and semiotic perspective. She has previously been associated with organisations such as OMA Rotterdam, INTACH Delhi and the TU Delft. Her current research includes a multidisciplinary project funded by the Leverhulme Trust, which brings together architects and crystallographers at Cardiff University to investigate what designers can learn from matter at the nanoscale.

P. Andrew Williams is a postdoctoral research chemist at Cardiff University. He completed a Masters in Chemistry at the University of Oxford prior to undertaking a PhD in solid-state chemistry with Professor Kenneth Harris at Cardiff University. His research has been based on the study of crystallization processes, the ability of molecules to form multiple different packing arrangements and the determination of crystal structures. Currently, he is involved in a collaborative project between crystallographers and architects.

Benson M. Kariuki has vast research experience in Solid State Chemistry with particular interest is the rationalization of relationship between structure and properties. He graduated from the University of Cambridge (PhD, 1990) and obtained postdoctoral and research fellowships at the Universities of Liverpool, Birmingham and University College London and a lectureship at Cardiff University .

Kenneth D. M. Harris graduated from the University of Cambridge (PhD; 1989), before holding academic positions in Physical Chemistry at St Andrews, UCL and Birmingham. He was appointed Distinguished Research Professor in Chemistry at Cardiff University in 2003. He has advanced new directions of research to understand structural properties of crystalline materials, and has developed novel experimental techniques to investigate these properties. His research has been recognized by several awards and prizes, and election to three national/international academies (Royal Society of Edinburgh, Learned Society of Wales, Academia Europaea). He has held appointments as Visiting Professor in Japan, France, USA, Spain and Taiwan.