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MATHEMATICS FOR MATERIALS

ABSTRACT
With the growing eagerness of the rapid advancement of computers, information science and mathematical science together with statistics and probability theory, the "data driven materials designs" has become a frequent idiom. In this paper, a few examples are briefly presented for the exploitation of mathematics used in the study of matter and materials and some rising collaborations are used.

KEYWORDS: *Disordered systems, Multi-scale hierarchical materials, Non-equilibrium materials, Carbon networks, Topological data analysis and Discrete geometry.*

1. INTRODUCTION

Mathematics has furnished the common language of science and technology since ancient times. Calculus is not only used to analyze shapes of objects but also motions according to the principle of the least action. The percept of probability was inserted in the 17^{th} century by Pierre de Fermat and Blaise Pascal. The modern probability theory was founded by Andrey Kolmogorov in the 20th century. Before the digital world arose in the cyber space, materials sciences had met with the discrete world. Deliberation of materials can be done as systems of hierarchical networks, which binds the continuous and discrete worlds. There are some excess requirements outside of the mathematical society for mathematical theories and apparatus that can describe the relationships between the continuous and discrete worlds. Congruently, at the end of the 20^{th} century, mathematics has enlarged the discrete world, such that in the cases of discrete group theory, discrete geometry and discrete geometrical analysis, with a concern in deepening mathematical theories. Here, a few examples are discussed regarding the applications of mathematics in the study of matter and materials and also some emerging collaborations are put forwarded [I].

2. MATHEMATICS FOR MATERIALS

The detailed account of how mathematics applied in different arenas are presented hereunder.

1.) Orders hidden in disordered system:

The structural formulae of covalently bonded compounds are graphs; they are known as constitutional graphs. The importance of graph theory for atoms/molecules/materials strikes up from the existence of isomerism. Example: C_3 H_7OH (See figure 1).

Atom – vertex; Bond – edge

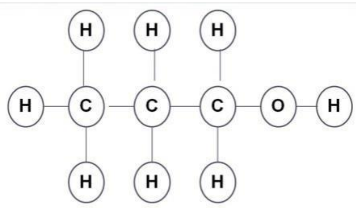

Figure 1: Atomic arrangement of C_3H_7OH.

Crystal lattices are defined as an abelian covering of a finite graph in the mathematical terminology and give a toy-portrait of the atomic arrangement of crystals [II, III].

Group theory is used to describe symmetries and periodicities in the atomic arrangements as well as it is used to find spectroscopy, M. O. Theory, etc.

The Method of applying group theory is discussed hereunder.

i. Find the point group of the molecule. All questions in quest to answer depend on the group to which the molecule belongs.

ii. Identify the basis set of the objects. It may include: a point (x, y, z); all 3N molecular motions; specific vibrations; a set of atomic orbitals, etc.
Use a vector (or orbital) on the molecule to represent each item. (n items = n vectors).
iii. Find the reducible representation recognizing symmetry of all items in the basis set.
iv. Reduce the representation to find the irreducible representation it contains.
(i.e. which row in the character table are represented). It provides the symmetries of the individual elements in the basis set.

2.) Topological functional elements:

Topology studies invariance of definite properties under continuous deformation, such as stretching, bending, or twisting, of the underlying geometry i.e. it affects physical properties of materials such as electronic conduction, charge and spin transport, light transmission, and response to a magnetic field. Topology is used to describe complex structures that are challenging under environmental change but have highly impressive properties simultaneously. Homology is used to count loops and holes and to study their connectivity. Topological data analysis is used to identify hidden orders in amorphous materials, polymers, or composite materials through collaborations. The index theorem for a non-commutative geometry or coarse geometry is used recently to understand topologically protected surface [IV].

3.) Discrete differential geometry for carbon networks:

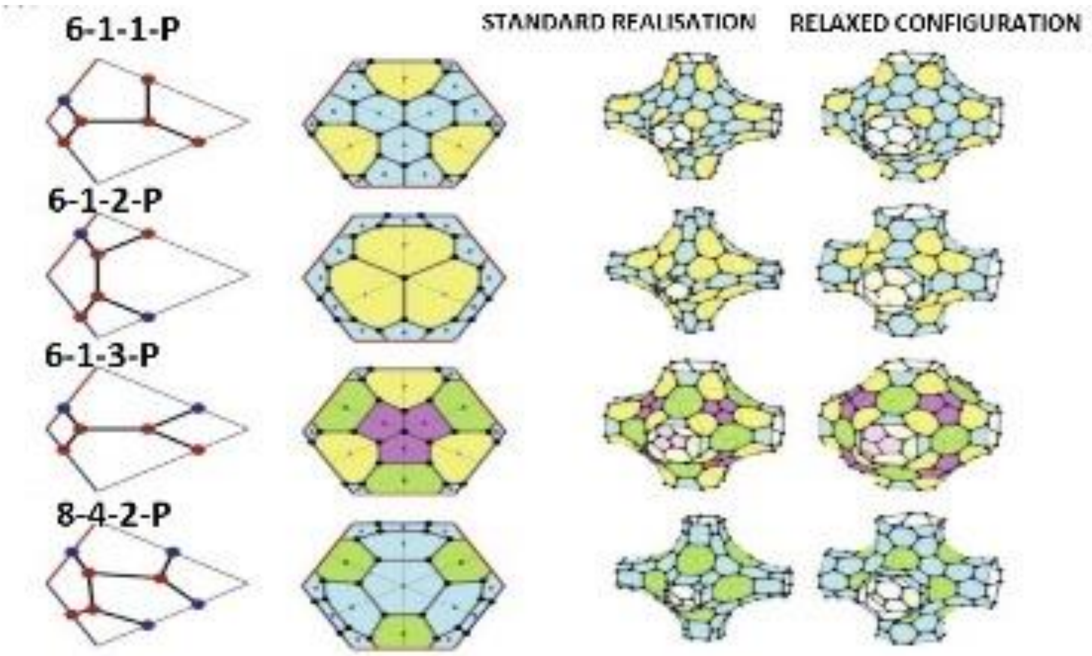

Figure 2: Mackay-like crystal.

In 2008, Toshikazu Sunada showed the beauty of diamond and K_4 lattice from a mathematical view and he challenged materials scientists to synthesize it [V]. There are many new structures synthesized by the researchers of organic chemistry for which there are no descriptions. This is a province in which anticipation of fertile collaborations will link materials scientists and mathematicians. Investigations are carried out since many years on carbon networks with negative curvatures (Mackay-like crystals as shown in figure 2) by applying notions in differential geometry [VI].

4.) Multi-scale hierarchal materials based on discrete geometrical analysis:

The innovative functional materials are formed by identifying and recognizing the complex multi-scale hierarchal structure in materials systems. Specific structure analysis and control at each level of hierarchy from the atomic or molecular scale can be carried out using any sophisticated apparatus with innovative technology. The discrete geometric analysis provides a link among scales and gives description of detailed geometric data. Using such advanced tools, the functional multi-scale hierarchical materials can be produced.

The graph is a chief and valuable tool in discrete geometrical analysis. Graph theory is used to investigate the 3D network structures and it can develop significant parameters, for example, related to material convey all the way through complex nanopore structures [VII]. As shown in figure 3, mathematics performs a task of wefts in textiles of material science and show the way to a board perspective ahead of the barriers isolating disciplines and discontinuities obtainable in hierarchy from micro to macro [VIII].

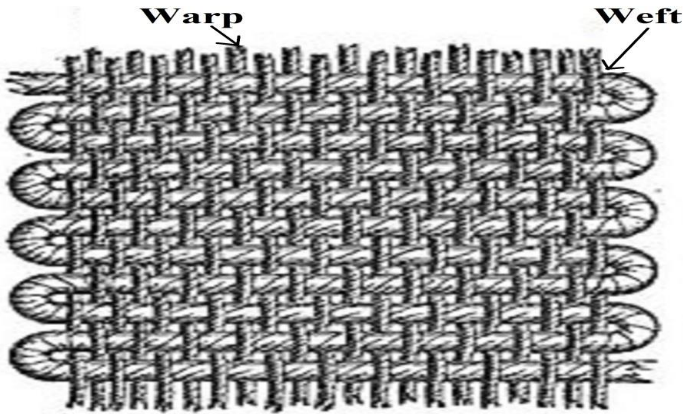

Figure 3: The role of mathematics presented as wefts in textiles.

5.) Non-equilibrium materials based on mathematical dynamical system:
On the origin of a mathematical dynamical system, clarifications for texture of dynamical structural can be formulated in non-equilibrium systems. This helps to manage non-equilibrium, inhomogeneous materials and to attain approved multiple functions for a given environment. Dynamical systems can be accompanied by treatment of stochastic processes. For example, in the amorphous glassy alloys, known to be the bulk metallic glasses, shear bands come into sight when continuous stress is applied but the timing of the appearance is more or less random and it is tricky to expect or control it. This is a trouble for the application of stochastic theory [VII].

CONCLUSION

Material science is, more or less, concerned with subdivision of research fields like metallurgy, polymer science, solid state physics and any other subdivided fields. It resulted in situation where nobody was able to broadly spot relations with subdivisions. It has now entered into the latest phase of growth. Integration of materials research enables us to find general methods secreted in the complex material system that establishes properties and functions. Mathematics is now ready to bid new tools to know materials as complex hierarchal systems. The Rich collaborations are now at our hands.

REFERENCES

I. M. Kotani and S. Ikeda, 2016, Mat. Inspired by Maths., Sci. & Tech. of Adv. Mater., Vol. 17 (1), pp. 253-259.
II. M. Kotani and T. Sunada, 2003, Spectral geometry of crystal lattices, Contemp. Math., Vol. 338, pp. 271–306.
III. M. Kotani and T. Sunada, 2000, Realization of Crystal Lattice Via Harmonic Maps., Trans Amer. Math. Soc., Vol. 353, pp. 1–20.
IV. G. M. Graf and M. Porta, 2013, Bulk-Edge correspondence for 2D topological insulators, Comm. Math. Phys., Vol. 324, pp. 851–895.
V. T. Sunada, 2008, Crystals that nature might miss creating, Not. Amer. Math. Soc., Vol. 55, pp.208–215.
VI. M. Tagami et al., 2014, Negatively curved cubic carbon crystals with octahedral symmetry, Carbon, Vol. 76, pp.266–274.
VII. D. V. Louzguine-Luzgin et al., 2013, On deformation behavior of a Ni-based BMG produced by flux treatment, J. alloys compd., Vol. 561, pp. 241–246.

VIII. S. Ikeda and M. Kotani, 2015, A new direction in maths. for mater. Sci., Springers Briefs in the maths. of materials, Vol.1, Tokyo : Springer.

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