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A mathematical challenge to a new phase of materials science

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Abstract

Recent challenges and some emerging results in the Mathematics-Materials Science are discussed.

Mathematics has developed in the interaction with other scientific fields and at the same time contributed their development by providing mathematical concepts and methods to formulate their problems. Examples are, say, Group theory to describe symmetries, partial differential equations to formulate mathematical models of phenomena in nature, probability theory to describe randomness. Since modern technology allows us to observe and control microscopic structure in materials and achieve useful functions, new mathematics are expected to bridge between microscopic structures and macroscopic properties. On the other hands mathematics to study discrete objects has developed much in the 21st century. Discrete Geometric Analysis is one of such attempts that bridge between discrete and continuum by putting emphasis on geometric viewpoints. When we consider materials as hierarchical networks; atom-atomic clusters-network of clusters-nanostructure-materials, we can apply recent development of Discrete Geometric Analysis.

Mathematics-Materials science collaboration has started at the Advanced Institute for Materials Research (AIMR), Tohoku University by setting the target projects: *"Non-equilibrium Materials based on Mathematical Dynamical Systems", "Topological Functional Materials", "Multi-Scale Hierarchical Materials based on Discrete Geometric Analysis"* under the WPI program by the MEXT. In the talk, some of emerging results obtained in the projects are presented to understand relations between structures and functions of materials in the universal language of mathematics.

More precisely, detections of hidden orders in amorphous like metallic glasses by using the Topological Data Analysis, topological phases in disorder systems by using the K-theory in noncommutative geometry, and descriptions of carbon networks and identification of continuum behind them by using discrete surface theory and convergences in the Gromov-Hausdorff topology are the examples we would like to discuss.

References

[1] Materials inspired by mathematics, Motoko Kotani and Susumu Ikeda, Science and Technology of Advanced Materials (STAM),17(1),(2016),253-259

[2] A new direction in mathematics for materials science, Susumu Ikeda, Motoko Kotani, Springer Briefs in the Mathematics of Materials, vol.1, Springer, 2015

[3]A discrete surface theory,M. Kotani, H. Naito, T. Omori 、Computer Aided Geometric Design, 58（2017）, 24-54

[4] Quantization of interface currents, Motoko Kotani, Hermann Schultz-Baldes, Carlos Villegas-Blas, Journal of Mathematical Physics 55/12(2014)

[5] Negatively curved cubic carbon crystals with octahedral symmetry, M. Tagami, Y. Liang, H. Naito, Y. Kawazoe, M. Kotani, Carbon76(2014), 266-274

[6] Stereoisomerism in nanohoops with heterogeneous biaryl linkages of E/Z- and R/S-geometries "Sarkar, Parantap; Sun, Zhe; Tokuhira, Toshiki; Kotani, Motoko; Sato, Sota; Isobe, Hiroyuki, ACS Cent. Sci., 2016, 2 (10), pp 740-747

[7] Structural chemistry of belt-shaped cyclonaphthylenes: Stereoisomerism, crystal structures and dynamics" Zhe Sun,Takuya Suenaga,Parantap Sarkar,Sota Sato,Motoko Kotani, Hiroyuki Isobe, Proc Natl Acad Sci 113(29):8109-14.

[8]Geometric frustration of icosahedron in metallic glasses, A. Hirata, L. J. Kang, T. Fujita, B. Klumov, K. Matsue, M. Kotani, A. R. Yavari, M. W. Chen, Science 341(6144),376-379

Appendix

URL: http://www.wpi-aimr.tohoku.ac.jp/