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Shuang Zhang  
*Dalian University of Technology, zhangshuangchn@mail.dlut.edu.cn*

Chuang Dong  
*Dalian University of Technology*

Peter Häussler  
*Chemnitz University of Technology*

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Spherical-periodic order in crystalline phases and relevant cluster-plus-glue-atom model for aperiodic crystals

Shuang Zhang¹, Chuang Dong¹, Peter Häussler²

¹Key Laboratory for Materials Modification by Laser, Ion and Electron Beams (Dalian University of Technology), Ministry of Education, Dalian 116024, China
²Physics Institute, Chemnitz University of Technology, 09107 Chemnitz, Germany

Email of communicating author: dong@dlut.edu.cn

It has been widely accepted that spherical-periodic order generally dominates disordered structure formation, such as liquid and amorphous states, where atoms tend to gather near spherically periodic shells according to Friedel oscillations. Here it is revealed that the spherical-periodic order is also hidden in crystalline structures through scrutinizing all binary bulk-glass-relevant phases, which further represents the common structural homology of crystalline states and aperiodic crystals. Among the multiple nearest-neighbor clusters developed from all the non-equivalent atomic sites in a given phase, there always exists a principal cluster, centered by which the spherical periodicity, both topologically and chemically, is the most distinct. Then the principal clusters plus specific glue atoms just constitute the short-range-order structural units shared by aperiodic crystals and the corresponding crystalline phases. This is the so-called cluster-plus-glue-atom model, formulated as [cluster](glue atom)₁ or ₃ for aperiodic crystals, where the cluster is a nearest-neighbor coordination polyhedron and the one or three glue atoms are situated between the clusters. In constructing the composition formulas of aperiodic crystals, the detailed procedures using the cluster-plus-glue-atom approach have already been established, which include: choosing the deep eutectic zones; selecting the corresponding crystalline phases; defining the principal clusters via the criteria such as spherical periodicity and cluster isolation degree; determining the glue atoms and therefore the cluster formulas; and substituting the basic binary formulas with similar elements to reach better alloy performances.

Keywords: spherical-periodic order, cluster-plus-glue-atom model, composition formulas, aperiodic crystals