

Cluster-based short-range-order structural model of aperiodic crystals and relevant binary eutectics

Chuang Dong, Shuang Zhang

Key Laboratory for Materials Modification by Laser, Ion and Electron Beams (Dalian University of Technology), Ministry of Education, Dalian 116024, China

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

Previously we have proposed the cluster-plus-glue-atom model for aperiodic crystals, by introducing a new description method based on the short-range-order structural units, which are considered to be shared by crystalline and disordered states from the view of structural homology. In this model, aperiodic crystals satisfy simple composition formulas [cluster](glue atom)_{1 or 3} with 24 valence electrons per unit formula, where the cluster is a nearest-neighbor coordination polyhedron and the one or three glue atoms are suited between the clusters. The detailed procedures using such a structural model to interpret binary aperiodic crystals and some typical multi-component ones have already been established, and the key steps mainly include the selection of principal clusters from the corresponding crystalline phases and the determination of glue atoms. Since aperiodic crystal formation is generally associated with eutectics, the cluster-plus-glue-atom model can also be applied into eutectic point interpretation, by assuming that a eutectic liquid consists of two subunits issued from the relevant eutectic phases, each being expressed by the cluster formula for aperiodic crystals. Then the structural unit is composed of two clusters from the relevant eutectic phases plus 2, 4 or 6 glue atoms. Such a dual-cluster formulism is well validated in all boron-containing (except those located at the extreme phase diagram ends) and in some commonly-encountered binary eutectics, with accuracies below 1 at.%. The dual-cluster formulas are generally formed with two distinctly different cluster types, with special cluster matching rules such as cuboctahedron plus capped trigonal prism and rhombidodecahedron plus octahedral antiprism.

Keywords: cluster-plus-glue-atom model, composition formulas, aperiodic crystals, binary eutectics