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An atomistic cluster alignment method to identify and characterize the local atomic structural order in liquids and glasses

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EXTENDED ABSTRACT: An atomistic cluster alignment method is developed to identify and characterize the local atomic structural order in liquids and glasses. With the "order mining" idea for structurally disordered systems, the method can detect the presence of any type of local order in the system and can quantify the structural similarity between a given set of templates and the aligned clusters in a systematic and unbiased manner. Moreover, population analysis can also be carried out for various types of clusters in the system. The advantages of the method in comparison with other previously developed analysis methods are illustrated by performing the structural analysis for four prototype systems (i.e., pure Al, pure Zr, $Zr_{35}Cu_{65}$, and $Zr_{36}Ni_{64}$). The results show that the cluster alignment method can identify various types of short-range orders (SROs) in these systems correctly while some of these SROs are difficult to capture by most of the currently available analysis methods (e.g., Voronoi tessellation method). Such a full three-dimensional atomistic analysis method is generic and can be applied to describe the magnitude and nature of noncrystalline ordering in many disordered systems.

Keywords： Atomistic Cluster Alignment Method

BIOGRAPHY

Xiaowei Fang graduated from University of Science and Technology of China, received his bachelor degree in physics from USTC in 2006, visited Iowa State University in 2008-2010, and received his PhD in physics from USTC in 2011.

From 2011 to 2016, he worked at Shenzhen Institute of Advanced Research of Guangqi, mainly responsible for product development and marketing of metamaterial structural parts and exoskeleton robots. Now he is the Vice General Manager of Hardware Center of iFLYTEK. His work is focusing on Human-robot interaction and industrial robotics applications.