Classification of Crystallographic Groups of Alloy Systems by Isomap and Modularity Methods

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Abstract: Crystallographic classification of microstructure is a very important issue in material science especially numerous data were generated by experiments or Molecular Dynamic (MD) simulations. Some analysis tools were purposed, such as coordination analysis and Honeycutt-Anderson (HA) pair analysis [1], however, to analyze these huge amounts of data is still quite difficult. Sometimes, crystallography prior knowledge of their structures is also desired in the classification procedures. Not only the task is very labor intensive but also the result is susceptible to errors and is usually lack of objectivity. In this study, we developed a computational workflow which can get characteristic quantities of microstructures and identify different crystal structures without prior knowledge of crystallography. These characteristic quantities (a.k.a. Characteristic Indexes) are, for example, coordination number, local ordering, and local coordinate information, etc. After Characteristic Indexes of local structures were obtained, isomap [2] and modularity [3] methods are applied to classify their structures and to get their structural phase diagrams. The isomap method can define the similarity between different crystal structures by geodesic paths in a high-dimensional data manifold as well as the modularity method can find the best community structure of classification by optimization, i.e., to maximize the intra module connections as many as possible and to minimize the inter module connections as few as possible. With these tools, we can obtain the atomic structure evolution of alloy system during deformation. This method is verified and is useful for the structural Identification of the simulations results.

References

1. Honeycutt, J. D., Andersen, H. C. (1987). Molecular dynamics study of melting and freezing of small Lennard-Jones clusters. *Journal of Physical Chemistry, 91(19),* 4950-4963.
2. Tenenbaum, J. B. (2000). A global geometric framework for nonlinear dimensionality reduction. *Science, 290,* 2319-2323.
3. Guimerà, Roger, Nunes Amaral, Luís A. (2005). Functional cartography of complex metabolic networks. *Nature, 435,* 895-900.

DOI: 10.32604/icces.2019.05401 www.techscience.com/icces