

Size and composition dependence of the frozen structures in Co-based bimetallic clusters

Guojian Li, Qiang Wang, Yongze Cao, Jiaojiao Du, Jicheng He

Summary

This paper studies the size-dependent freezing of Co, Co-Ni, and Co-Cu clusters by using molecular dynamics with a general embedded atom method. There is size effect occurs in these three types of clusters. The clusters with large sizes always freeze to form their bulk-like structures. However, the frozen structures for small sizes are generally related to their compositions. The icosahedral clusters are formed for Co clusters (for 3.2 nm diameter) and also for Co-Ni clusters but at a larger size range (for 4.08 nm). Upon Co-Cu clusters, decahedral structure is obtained for small size (for 2.47 nm). The released energy induced the structural transformation plays a key role in the frozen structures. These results indicate that the preformed clusters with special structures can be tuned by controlling their compositions and sizes.

