

Abstract Submitted  
for the MAR15 Meeting of  
The American Physical Society

**Melting behavior of metallic clusters: An order parameter by instantaneous normal modes** TEN-MING WU, Institute of Physics, National Chiao-Tung University — In this paper, we investigated the melting behaviors of  $\text{Ag}_{17}\text{Cu}_2$  and  $\text{Ag}_{14}$  metallic clusters, which were generated by isothermal Brownian-type molecular dynamics simulation with the empirical many-body Gupta potentials, from low to high temperatures. For the two clusters, the temperature variation in the specific heat exhibited a maximum at a temperature, which was defined as the cluster melting temperature. However, an additional prepeak at a lower temperature was found in the specific heat variation of  $\text{Ag}_{14}$  but no prepeak was found in that of  $\text{Ag}_{17}\text{Cu}_2$ . The instantaneous normal mode (INM) analysis was used to dissect dynamics of the two clusters. A new order parameter associated with a cluster was proposed to describe the melting behaviors of the cluster; the order parameter can be defined using either the INM vibrational density of states or three orthogonal eigenvectors describing the rotational motions of the cluster by considering it as a rigid body. For the two metallic clusters studied, our results showed the mutual agreement for the order parameter defined by the two methods. The interpretation by the order parameter for the melting transition of a cluster was consistent with the temperature variation in the specific heat of the cluster. Furthermore, the new order parameter provided a connection between the melting of clusters and the concept of broken symmetry, which was successfully applied for understanding the melting transition of bulk systems.

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Date submitted: 13 Nov 2014

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