NREL Scientists Reveal Origin of Diverse Melting Behaviors of Aluminum Nanoclusters

Research reveals active role of cluster symmetries on the size-sensitive, diverse melting behaviors of metallic nanoclusters, providing insight to understanding phase changes of nanoparticles for thermal energy storage.

Unlike macroscopic bulk materials, intermediate-sized nanoclusters with around 55 atoms inherently exhibit size-sensitive melting changes: adding just a single atom to a nanocluster can cause a dramatic change in melting behavior. Microscopic understanding of thermal behaviors of metal nanoclusters is important for nanoscale catalysis and thermal energy storage applications. However, it is a challenge to obtain a structural interpretation at the atomic level from measured thermodynamic quantities such as heat capacity.

Using *ab initio* molecular dynamics simulations, scientists at the National Renewable Energy Laboratory (NREL) revealed a clear correlation between the diverse melting behaviors of aluminum nanoclusters and cluster core symmetries. These simulations reproduced, for the first time, the size-sensitive heat capacities of aluminum nanoclusters, which exhibit several distinctive shapes associated with the diverse melting behaviors of the clusters. The size-dependent, diverse melting behaviors of the aluminum clusters are attributed to the reduced symmetry (from Td → D2d → Cs) with increasing the cluster sizes and can be used to help design thermal storage materials.

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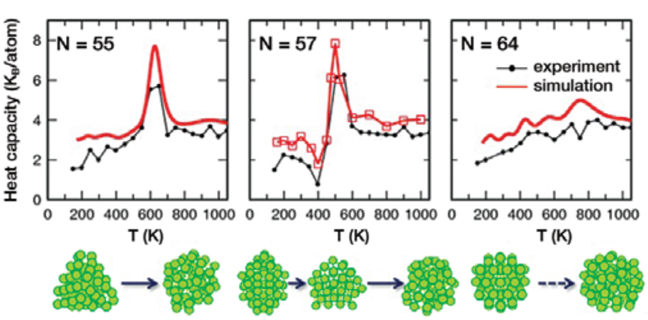
Reference: Kang, J.; Wei, S–H.; Kim, Y–H. "Origin of the Diverse Melting Behaviors of Intermediate-Size Nanoclusters: Theoretical Study of AlN (N=51-58, 64)." *J. Am. Chem. Soc.* **132**, 18287 (2010).



Simulated heat capacities (red lines) from MD simulations are compared with experimental data (black dots and lines) for AlN clusters with N = 55, 57, and 64, respectively.

Key Research Results

Achievement

NREL scientists have revealed the active role of cluster symmetries on the size-sensitive, diverse melting behaviors of metallic nanoclusters.

Key Result

This research provides insight to understanding phase changes of nanoparticles for thermal energy storage.

Potential Impact

Microscopic understanding of thermal behaviors of metal nanoclusters is important for nanoscale catalysis and thermal energy storage applications.

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