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Monte Carlo study on the melting process of small metal clusters

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Cluster science has focused on the size-dependent evolution of solid-state properties in systems where chemical bonding and electron delocalization are fairly strong. While this subject remains poorly understood, clusters of intermediate size are often found to have hybrid properties characteristic of neither the molecular nor bulk solid-state limits. The physical properties of very small clusters generally differ from those of the free atoms or molecules themselves, as well as from the properties of the bulk solids. The study of the stability of individual clusters as a function of temperature, and in particular "phase transformation", has raised some interests.

We have simulated the melting process of a small clusters ($5 \leq n \leq 25$) consisted of single element (Ni, Pd, Pt, Cu, Ag, Au, Pb, and Al). We will discuss, from the microscopic view point, the temperature and types of phase transitions and also the process of structural rearrangements.