

Three-Dimensional Atomic Structure and Surface Dynamics of Size-Selected Au₉₂₃ Clusters

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The activity and selectivity of nanocluster catalysts depend on their size, shape and atomic configuration, so the structural characterization of the nanoclusters is fundamentally important for understanding the catalytic performance [1-3]. Aberration-corrected scanning transmission electron microscopy (STEM) has been successfully used in revealing the three-dimensional structures of size-selected Au₃₀₉ clusters [4]. In this paper, we report the structural determination of size-selected, magic number Au₉₂₃ clusters as well as revealing surface atomic dynamics relevant to the catalytic activity.

Size-selected Au₉₂₃ clusters were deposited with a radio frequency magnetron-sputtering, gas aggregation cluster beam source. A novel, lateral time-of-flight mass filter was used to obtain the size-selection with a precision of $M/\Delta M=20$ [5-7]. The high angle annular dark field (HAADF) - STEM investigation was performed in a JEOL2100F instrument with spherical aberration corrector (CEOS GmbH). Sub-Å resolution can be reached under optimized conditions.

Fig. 1 shows representative HAADF-STEM images of the Au₉₂₃ clusters. Two kinds of structure were observed in the clusters, specifically, cuboctahedral, shown in fig. 1 (a), and decahedral, shown in fig. 1(b). Structural statistics from more than 40 clusters show that ~ 85% are cuboctahedral or FCC-like twin structures, consistent with previous theoretical calculations of the total potential energy [4].

Fig. 2 shows two consecutive HAADF-STEM images obtained in serial-acquisition experiments on the same particle. The particle appears quite stable under the electron beam, and neither obvious change of orientation nor particle reconstruction was found. However, comparing the two images, we find that the number and position of the surface atoms display significant changes. In fig. 2(a), for example, facet A shows three atomic columns, and facet B 2 atomic columns. By contrast, facet A in fig. 2(b) exhibits only 1 atomic columns, and facet B 5 atomic columns. It seems that some adatoms have moved from facet A to B. Such weakly bound surface atoms present interesting possibilities as active site for catalytic reactions. The dependence of the surface atomic dynamics on electron beam current will also be discussed.

References

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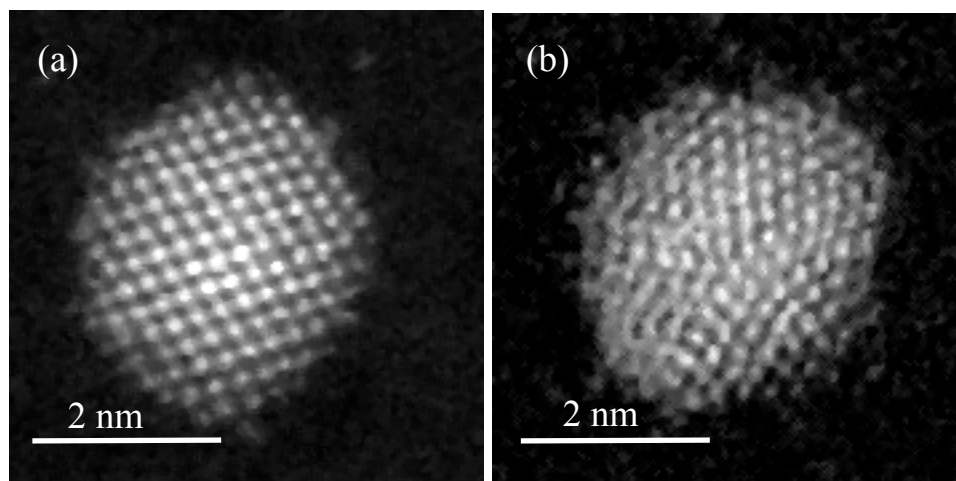


FIG. 1. Representative HAADF-STEM images of size-selected Au₉₂₃ clusters. (a) Cuboctahedral structure, (b) decahedral structure.

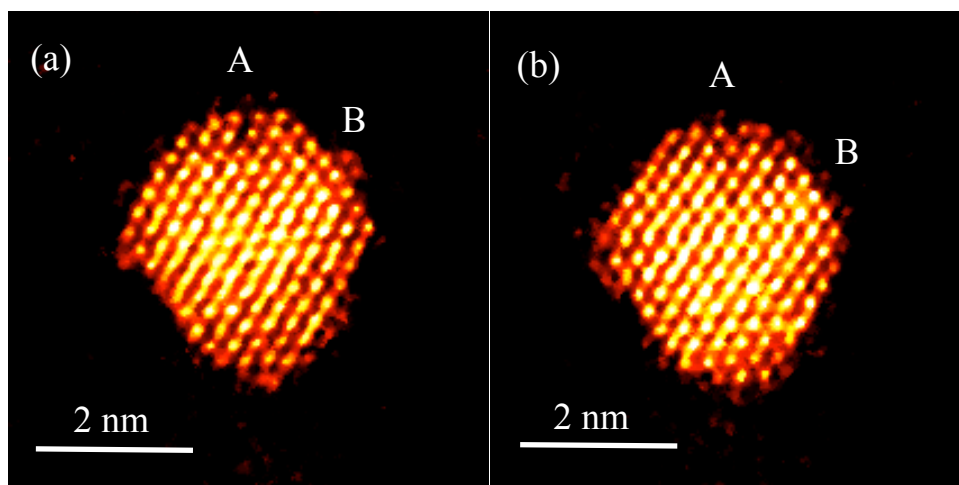


FIG. 2. Serial-acquisition of HAADF-STEM images of Au₉₂₃ clusters with a speed of 6 s/frame. (a) and (b) are two consecutive frames.