Electronic Supplementary Material (ESI) for Nanoscale.

SUPPORTING INFORMATION

Thermally activated microstructural evolution of metallic heterophase nanoparticles: Insights from molecular dynamics simulations

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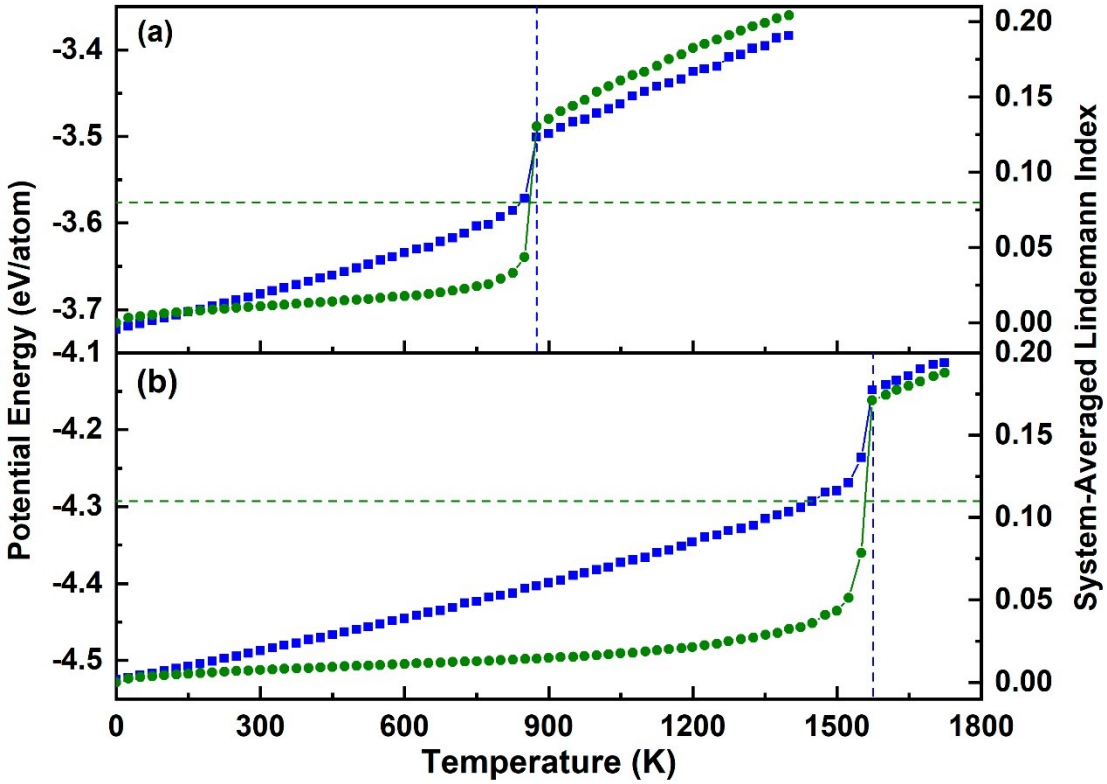

Fig. S1. Temperature-dependent potential energy and Lindemann index of (a) Au and (b) Co single-phase nanoparticles. The blue and olive solid lines denote the potential energy and Lindemann index, respectively. The vertical and horizontal dashed lines respectively represent the melting temperature of the corresponding nanoparticle and the critical value of Lindemann index.

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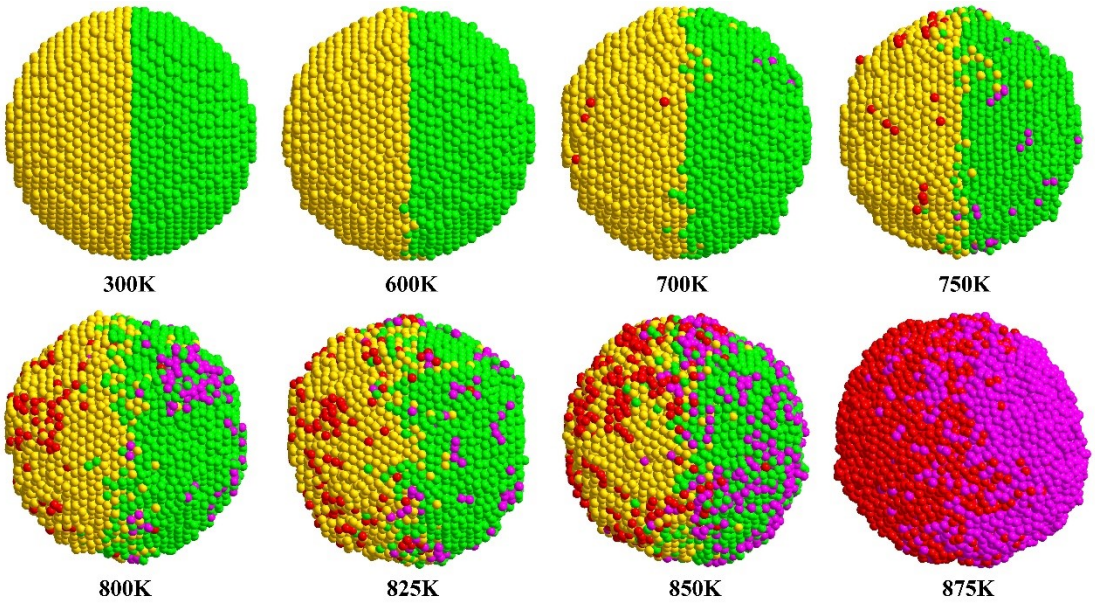

Fig. S2. Atomistic snapshots of Au heterophase nanoparticle at eight representative temperatures. Coloring in these snapshots denotes atomic type: yellow, non-Lindemann Au atoms initially located in *fcc* domain; red, Lindemann Au atoms initially located in *fcc* domain; green, non-Lindemann Au atoms initially located in *hcp* domain; pink, Lindemann Au atoms initially located in *hcp* domain.

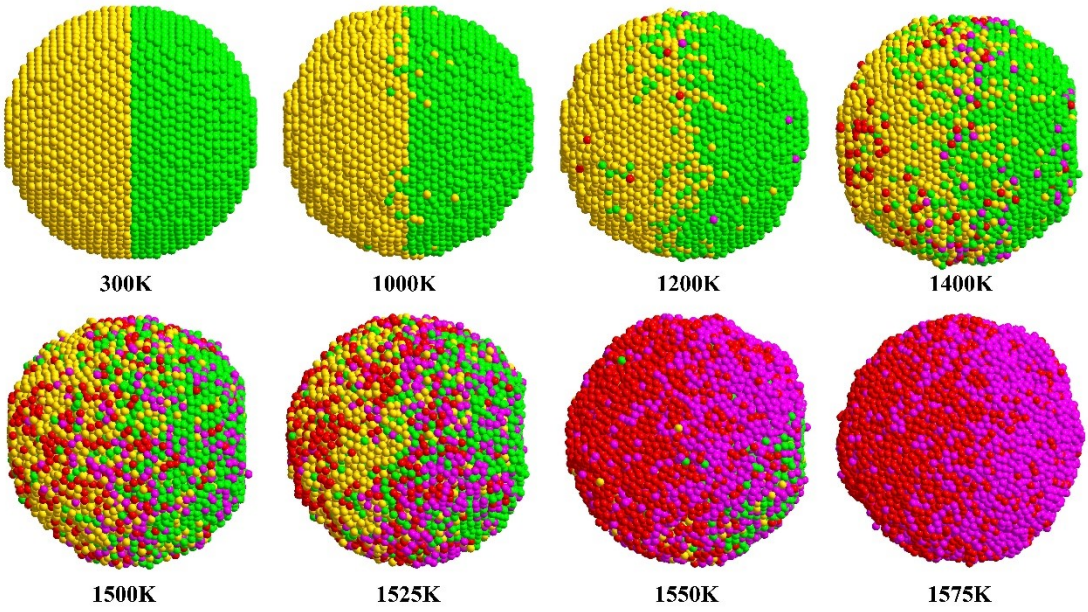

Fig. S3. Atomistic snapshots of Co heterophase nanoparticle at eight representative temperatures. Coloring in these snapshots denotes atomic type: yellow, non-Lindemann Co atoms initially located in *fcc* domain; red, Lindemann Co atoms initially located in *fcc* domain; green, non-Lindemann Co atoms initially located in *hcp* domain; pink, Lindemann Co atoms initially located in *hcp* domain.