Structure of a seeded palladium nanoparticle and its dynamics during the hydride phase transformation

Ana F. Suzana\textsuperscript{1,*}, Longlong Wu\textsuperscript{1}, Tadesse A. Assefa\textsuperscript{1}, Benjamin P. Williams\textsuperscript{2}, Ross Harder\textsuperscript{3}, Wonsuk Cha\textsuperscript{3}, Chun-Hong Kuo\textsuperscript{4}, Chia-Kuang Tsung\textsuperscript{2} and Ian K. Robinson\textsuperscript{1,5,*}

\textsuperscript{1} Condensed Matter Physics and Materials Science Department, Brookhaven National Laboratory, Upton, NY 11793, USA
\textsuperscript{2} Department of Chemistry, Merkert Chemistry Center, Boston College, Chestnut Hill, MA 02467, USA
\textsuperscript{3} Advanced Photon Source, Argonne National Laboratory, Lemont, IL 60439, USA
\textsuperscript{4} Institute of Chemistry, Academia Sinica, Taipei 11529, Taiwan
\textsuperscript{5} London Centre for Nanotechnology, University College London, London WC1E 6BT, UK

Supplementary information
Supplementary Figure 1. Electron microscopy images of the seed precursor and the final nanocrystal. (a) Bright-field TEM images of the Pd seeds. The scale bar in the inset panel is 20 nm. (b) SEM image of the TiO₂-coated Pd nanocrystals studied in the BCDI experiment.
Supplementary Figure 2. The original wrapped real phase for the nanoparticle measured under pristine conditions. The [111] direction is shown as the black arrow.

Supplementary Figure 3. Displacement distribution map shown as cross-section views for the nanoparticle measured under pristine conditions. (a) Spatial positions of the cross-sections (1-5) shown in (b). The volume particle is displayed as a semi-transparent isosurface. The [111] direction is shown as the black arrow in (a) and in all cross-sections in (b).
**Supplementary Figure 4.** Finite element model results using a symmetric octahedron. Cross-section of the model (left) taken in the x direction, corresponding to the direction of the Q vector in the experimental data. Cross-sectional view (right) taken in the same position as cross-section number 1 shown in Fig. 4.

**Supplementary Figure 5.** Plot showing the integrated intensity of the 3D data as a function of hydrogen exposure time. The first scan was discarded and the following ones (from time = 4-40 min), representing states I, II and III, were averaged in groups to improve statistics.
Supplementary Figure 6. Reconstructed wrapped phases for states I-III shown in Fig. 5. The nanoparticle was measured under a flux of hydrogen ($p_{H_2} = 4.410 \text{ Pa}$) through the sample to induce the $\alpha$-$\beta$ phase transformation.