Electronic Supplementary Information:

Sinter-free phase conversion and scanning transmission electron microscopy of FePt nanoparticle monolayers

Aaron C. Johnston-Peck, ^a Giovanna Scarel, ‡^b Junwei Wang,
§^a Gregory N. Parsons, ^b and Joseph B. Tracy
*^a

^a Department of Materials Science and Engineering, North Carolina State University, Raleigh, NC, 27695, USA. E-mail: jbtracy@ncsu.edu
 ^b Department of Chemical and Biomolecular Engineering, North Carolina State University, Raleigh, NC, 27695, USA
 ‡ Current Address: Department of Physics and Astronomy, James Madison University, Harrisonburg, VA 22807, USA
 § Current Address: Department of Materials Science and Engineering, Rensselaer Polytechnic Institute, Troy, NY 12180, USA

Representative transmission electron microscopy images of the as-synthesized nanoparticles with selected-area electron diffraction:



Figure S-1. Representative TEM image of 4.2 nm FePt nanoparticles.



Figure S-2. Representative TEM image of 4.9 nm FePt nanoparticles.



Figure S-3. Representative TEM image of 5.9 nm FePt nanoparticles.

Energy dispersive X-ray spectra:



Figure S-4. EDS spectrum for 4.2 nm FePt nanoparticles.



Figure S-5. EDS spectrum for 4.9 nm FePt nanoparticles.



Figure S-6. EDS spectrum for 5.9 nm FePt nanoparticles.

Additional TEM image:

Figure S-7. TEM image of a spin cast array of a partial multilayer of 4.2 nm diameter FePt nanoparticles.

Additional Z-contrast STEM images:

Figure S-8. HAADF-STEM images used in Figure 6, before noise filtering.

Figure S-9. HAADF-STEM images used in Figure 7, before noise filtering.

Figure S-10. HAADF-STEM images used in Figure 8, before noise filtering.

Figure S-11. (a-b) Filtered and (c-d) the original, unfiltered HAADF-STEM images showing the presence of the FePt₃ phase forming on the edges of the nanoparticles.

Details of Z-contrast STEM image simulation:

Images were simulated using QSTEM, a program written by Chistoph Koch that is based in Matlab and uses a multislice algorithm to compute the wave function at the exit surface of the crystal. The .cfg files used to generate the models employed in the simulation are as follows:

FePt L1₀:

```
Number of particles = 4
A = 1.0 Angstrom (basic length-scale)
H0(1,1) = 3.852 A #
```

```
HO(1,2) = 0 A
HO(1,3) = 0 A
HO(2,1) = 0 A #
H0(2,2) = 3.822 A
                     #
HO(2,3) = 0 A
HO(3, 1) = 0 A
HO(3,2) = 0 A
HO(3,3) = 3.713 A #
.NO VELOCITY.
entry count = 5
56
Fe
 0.50
        0.00
                  0.50 0.35 1
0.00
         0.50
                  0.50 0.35 1
195
Ρt
      0.00 0.00 0.37 1
0.50 0.00 0.37 1
 0.00
 0.50
```

FePt L1₂:

```
Number of particles = 4
A = 1.0 Angstrom (basic length-scale)
HO(1,1) = 3.877 A \#
HO(1,2) = 0 A
HO(1,3) = 0 A
HO(2,1) = 0 A #
HO(2,2) = 3.877 A
                   #
HO(2,3) = 0 A
HO(3,1) = 0 A
HO(3,2) = 0 A
HO(3,3) = 3.877 A #
.NO VELOCITY.
entry count = 5
56
Fe
       0.00 0.50 0.35 1
0.50
195
Ρt
0.00 0.00 0.00 0.37 1
0.50
        0.50
                0.00 0.37 1
0.00
        0.50
                0.50 0.37 1
```

The lattice parameters are from JCPDS files (43-1359 and 29-716), and the Debye-Waller factors from the literature.¹ A $10 \times 10 \times 15$ unit cell box was simulated with zero tilt in all directions. A scan window of $15 \text{ Å} \times 15 \text{ Å}$ and a scan length of 25 pixels in each direction were chosen. The model was sliced into two horizontal slabs with 30 slices per slab. Microscope parameters were then selected that would *approximately* mimic the experimental setup used on the JEOL 2010F: voltage: 200 kV, defocus: -43.4 mm, Cs: 0.5 mm, temperature: 300 K, Cc: 1.1 mm, convergence angle: 8.5 mrad, dE: 0.8 eV, dwell time: 15.7 µs, and detector inner and outer angles: 60 and 200 mrad, respectively. A total of 30 thermal diffuse scattering (TDS) configurations were averaged to compute the final image that was viewed with an oversampling of 7 and an assumed source

size of 1.3 Å. The final image was from a ~ 3.7 nm thick section, and Poisson (shot) noise was added.

1. Sears, V. F.; Shelley, S. A., Debye-Waller Factor for Elemental Crystals. *Acta Crystallogr. Sect. A* **1991**, *47*, 441-446.