In Situ TEM Observation of Epitaxy-induced NaCl Phase Transformation on the Au Nanowire Substrate

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Transmission electron microscopy (TEM) is a powerful tool to investigate dynamic behaviors of materials on the atomic scale by means of either ex-situ [1, 2] or in-situ [3]. Thanks to the significant advances in the microscopic technologies, a large number of interesting phenomena are revealed clearly and can be explained in details upon direct TEM observations [4]. On the other hand, epitaxy-induced structural phase transformation of NaCl was revealed successfully by the calculation in the 1980s [5], however, there has been very rare sharp evidence captured by TEM to support this prediction. Here, we report the in-situ TEM observation of NaCl phase transformation catalyzed by Au nanowires, which act as a face-centered cubic (fcc) substrate.

Figure 1(a) shows a representative TEM image where NaCl nano-crystallite (highlighted by the red arrow and box) localizes closely to an individual Au nanowire. The measured latticed distance is 2.86 Å in Figure 1(b), which is consistent with NaCl (001) [6]. The corresponding FFT pattern shows a cubic symmetry, suggesting the [100]-oriented NaCl. The schematic illustration of 3-D NaCl cubic structure is shown in Figure 1(d).

With electron irradiation, we find NaCl nano-crystallite moves towards the nanowire and ultimately, they get attached as shown in Figure 2(a). NaCl maintains its cubic structure until the attachment. Upon the contact, it starts to get wetted on the Au nanowire, as it becomes thinner in the transverse direction and longer in the longitudinal direction of the nanowire. More interestingly, we observe the upper part of NaCl nano-crystallite gradually transforms into fcc structure while the structure of the bottom part remains unchanged, as presented in Figure 2(f). Grain boundary between fcc-NaCl and cubic-NaCl can be clearly observed. Higher magnification of the fcc region is shown in Figure 2(g), which demonstrates the epitaxy relation of fcc-NaCl with the Au nanowire. The FFT pattern shows a hexagonal symmetry, as identified from Figure (h), which features the successful transformation from the cubic to fcc. As NaCl is composed of Na⁺ and Cl⁻, its fcc structure is identical to the ZnS crystalline structure, one of the representative crystalline structures in compounds.

The discussions will be extended to the dynamic activities of NaCl under the electron irradiation. Epitaxy relation will be supported by more evidence. We will also discuss the mechanism for the epitaxy-induced phase transformation of NaCl. This work will enhance the understanding of the crystal phase transformations under particular and extreme conditions.





Figure 1. (a) A representative TEM image of NaCl nanocrystallite and Au nanowire. (b) High-resolution image revealing the lattice distance of NaCl (100) ~2.86 Å. (c) The corresponding FFT from (b) showing NaCl-type structure. (d) The modeling structure of NaCl.



Figure 2. (a)-(f) Time-lapsed TEM images of NaCl structure modified from NaCl-type to ZnS-type (face-centered). (g) The high-resolution TEM image of the face-centered NaCl together with Au nanowire. (h) The corresponding FFT shows a hexgonal pattern, which confirms the transformation.

References

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