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Grain Boundaries and Anti-Phase Boundaries in $Ba_{1.015}Zr_{0.8-x}Ce_{0.2}Y_xO_3$ Proton Conductors

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Proton conducting ceramics[1] play a key role in clean hydrogen-based electricity generation processes. Protonic ceramic fuel cells (PCFC) are promising due to lower operating temperature and absence of fuel dilution (allowing high fuel utilization). We focus on $Ba(Ce,Zr,Y)O_3$ electrolyte materials owing to its very high bulk proton conductivity and excellent chemical stability at temperatures of 400 ~ 700 ºC. However, grain boundaries (GBs) exhibit a blocking character, and both bulk and grain boundary conductivity are very sensitive to the exact cation composition (ratio of Ba to (Ce+Zr+Y)).

We studied the atomic-scale composition and structure of both the bulk and GBs of $Ba_{1.015}Zr_{0.8-x}Ce_{0.2}Y_xO_3$ samples (x = 0.05 and 0.136, sintered by spark plasma sintering (SPS) and annealed at 1500 °C) by aberration-corrected analytical TEM techniques. For both samples, quantitative EDS of GBs showed a decreased density for all elements. The relative concentrations increase for Ba and Y, and decrease for Zr and O. Two types of Ba-rich anti-phase boundaries (APBs), as shown in Figure 1 and Figure 2, were observed in the bulk region by high-angle annular dark-field (HAADF) imaging, which we denote as APB-1 and APB-2. APB-1 has a phase shift of half a {100} plane distance along [100] direction with BaO planes as the connecting planes. APB-2 has a phase shift between 0 to half a {100} plane distance also along [100] direction. Different to APB-1, Ce- and Y-rich (Zr,Ce,Y)O planes marked by arrows in Figure 2 are present between the neighboring BaO planes, where Ce shows reduced valence. APB-1s are more frequent for x = 0.05 samples, while x = 0.136 samples show more APB-2s. The importance of APBs to accommodate cation non-stoichiometries will be discussed. More details and their correlation to proton conductivity will be presented [2].

References:

[1] KD Kreuer, Annu. Rev. Mater. Res. **33** (2003), p. 333.
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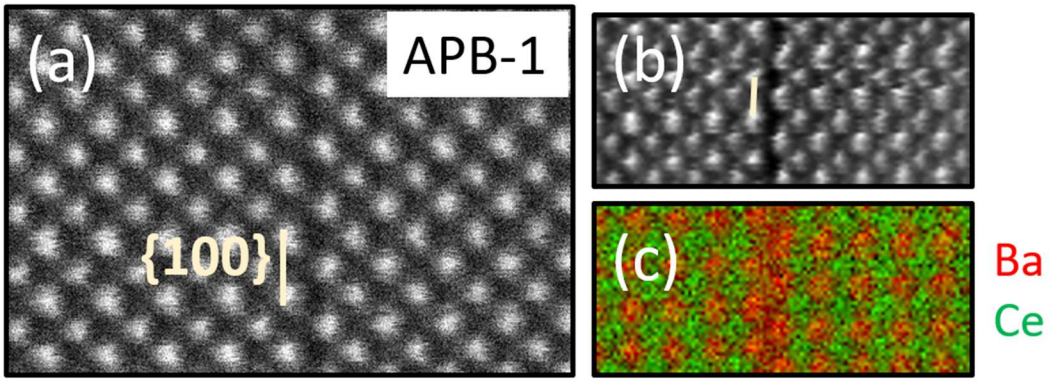

Figure 1. (a) HAADF image of APB-1; (b) simultaneously acquired ADF image and (c) EEL spectrum images using Ba-M (red) and Ce-M (green) absorption edges.

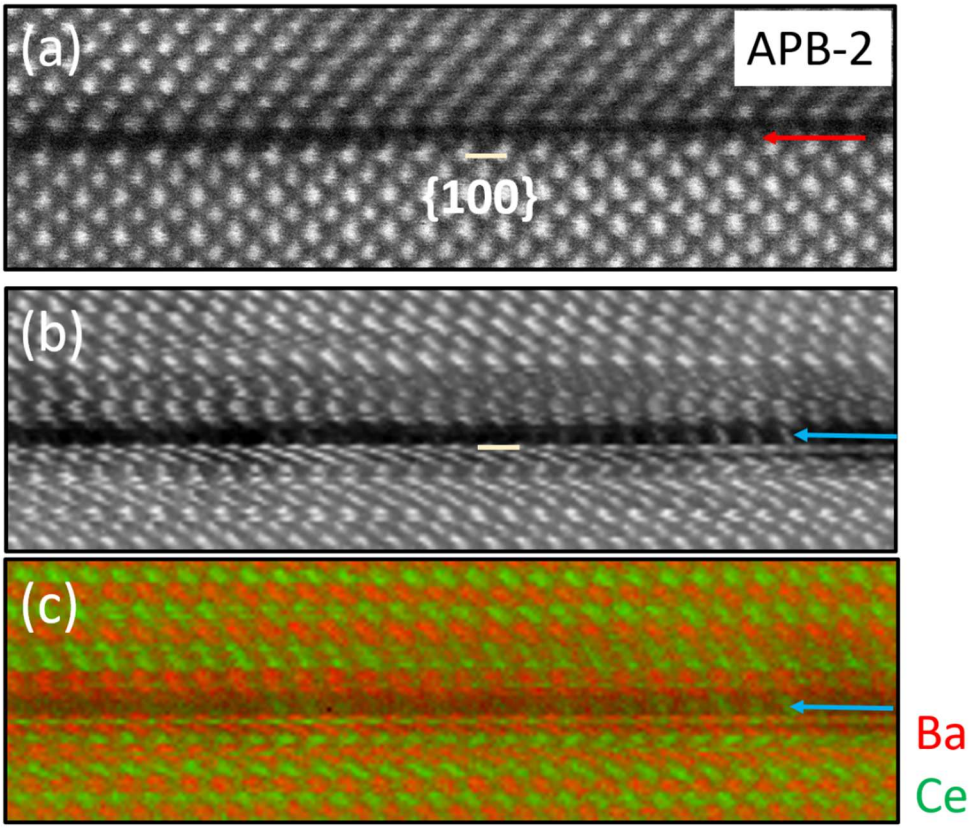

Figure 2. (a) HAADF image of APB-2; (b) simultaneously acquired ADF image and (c) EEL spectrum images using Ba-M (red) and Ce-M (green) absorption edges.

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