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Anti-Site Defects in Perovskite $YAlO_3$:Ce Using Aberration-Corrected STEM

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The aluminate perovskites $YAlO_3$ have been identified as potential scintillator materials due to their high light output and short decay time. However, the performance of $YAlO_3$ is still low. Despite the promising optical properties of $YAlO_3$, it has been proposed that their potential as scintillators has not been fully realized[1]. Recently, the focus has been on carrier traps as the limiting factor in the performance of $YAlO_3$, but the nature of these traps has not been identified. An investigation using first-principles calculations suggested that anti-site defects in which B-site Aluminum and A-site Yttrium are interchanged have a lower energy than Shottky or Frenkel defects[2,3]. Despite numerous studies, there is still no direct evidence to show the existence of anti-site defects.

We have used a fifth-order aberration-corrected Nion UltraSTEM200 scanning transmission electron microscope to investigate the local atomic structure of $YAlO_3$ doped with 0.1% Ce. $YAlO_3:Ce^{3+}$ are expected to have both types of cation anti-site defects (Al on the Y site and Y on the Al site). High-angle annular dark-field (HAADF) imaging was used to detect the presence of anti-site defects in $YAlO_3:Ce^{3+}$.

A typical HAADF image from $YAlO_3:Ce^{3+}$ is seen in Figure1b along with an image simulation based on the multi-slice method. The image was obtained at 200 kV using a probe convergence angle of 30 mrad. We can see some B-sites Al+O columns with brighter intensity as indicated by white circles and a blue arrow in Figure1b. And we also can see an A-site column with reduced intensity as indicated by a red arrow in Figure1b and as shown line profile in Figure 2. To interpret these intensity variations, HAADF image simulations using a structure with between 0-10% Y on the Al B-site and 0-10% Al on the A-site Y were performed. As shown in Figure 2, the experimental and simulated intensities at A-sites and B-sites with and without 10% anti-site defects are in good agreement. Additional details on these $YAlO_3$:Ce crystals provided by DFT calculations and optical property measurements will be discussed.

References

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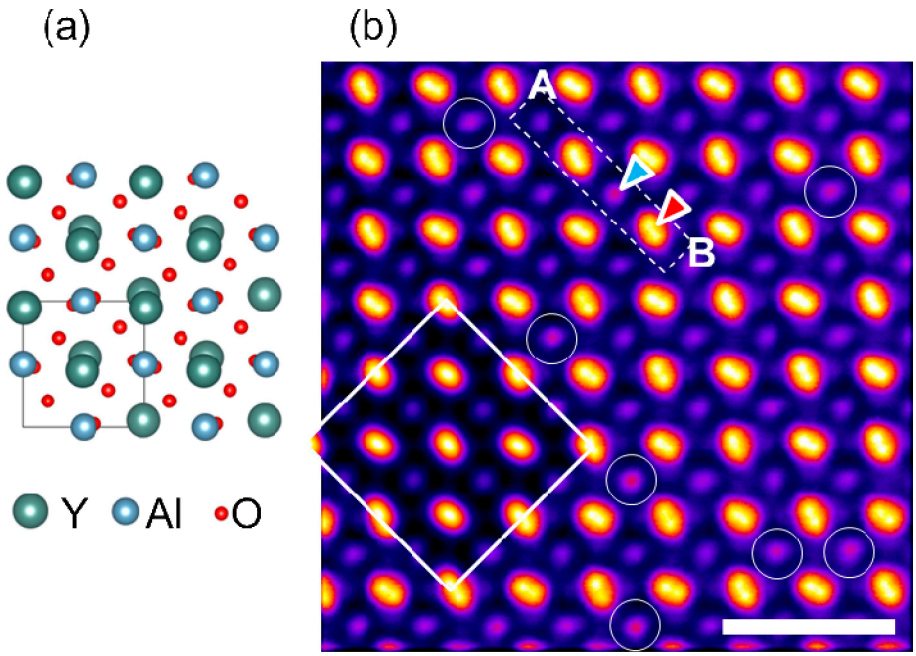

Figure 1. (a) Crystal structure of $YAlO_3$ viewed along <010> axis. (b) HAADF image obtained with detector ranges 60-200 mrad. Simulated image (HREM Inc.) using the structure of Fig.1a is inserted in the lower left side of the image. Scale bar: 1nm.

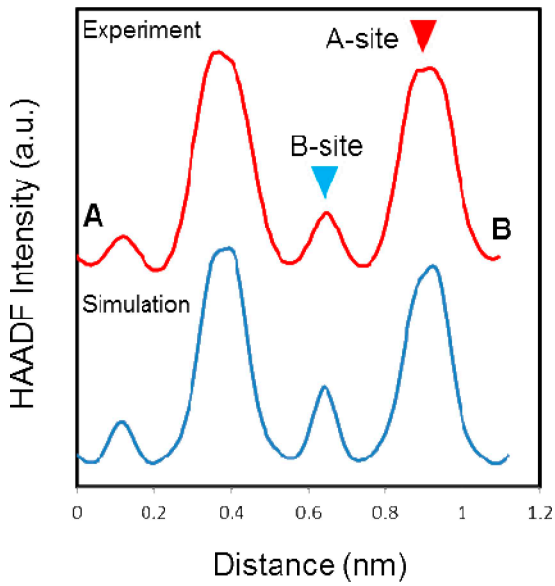

Figure 2. Red line profile along A-B indicated in Fig.1b, showing the experimental intensity of A-and B- sites. Blue line profile of simulated result obtained by using a structure with 10% Y on the B-site and 10% Al on the A-site Y. Simulated profiles calculated for specimen thicknesses of 10 nm.

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