In-Situ Neutron Powder Diffraction Study on In-Doped $BaCeO_3$

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$BaCeO_3$ is an electronic insulator and proton conductor making it a feasible a candidate for solid state proton electrolyte applications in fuel cells.[1] Previous neutron scattering studies by Knight indicated a sequence of phase transitions from orthorhombic (*Pnma* → *Imma*) via rhombohedral (*R-3c*) to a cubic (*Pm-3m*) structure at high temperature.[2] The orthorhombic structures are shown in figure 1. We are interested in In^{3+} doped analogues of $BaCeO_3$ which are intermediates for indium doped CeO_2 for oxidize ion conduction applications. Since powder X-ray diffraction experiments cannot identify the *Pnma* to *Imma* phase transition, this transition was investigated for $BaCe_{0.9}In_{0.1}O_3$, $BaCe_{0.8}In_{0.2}O_3$ using the neutron powder diffractometer C2 at the CNBC. Figure 2 shows the neutron powder diffractograms for $BaCe_{0.9}In_{0.1}O_3$ and $BaCe_{0.8}In_{0.2}O_3$ between 25˚C and 450˚C and clearly show the disappearance of the (122) and (102) reflections consistent with the phase transition from *Pnma* to *Imma* below 200˚C. This finding is in agreement with the previous studies by Knight[2] on the undoped $BaCeO_3$ structure. Indium doping does not have a profound impact on the room temperature structure and the *Pnma* to *Imma* phase transition.[3]

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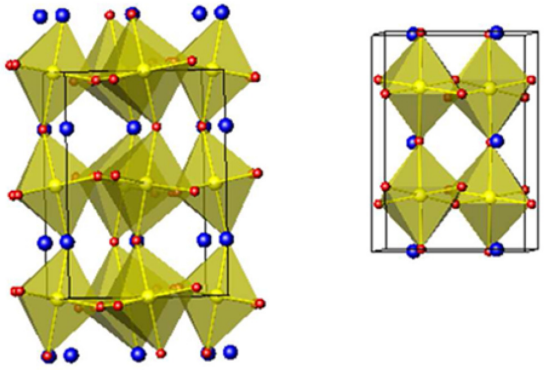

Figure 1: $BaCeO_3$ orthorhombic structures. Blue = Ba^{2+}, yellow = Ce^{4+}, red = O^{2-}. Left structure: $BaCeO_3$ in space group *Pnma*. Right structure: $BaCeO_3$ in space group *Imma*.

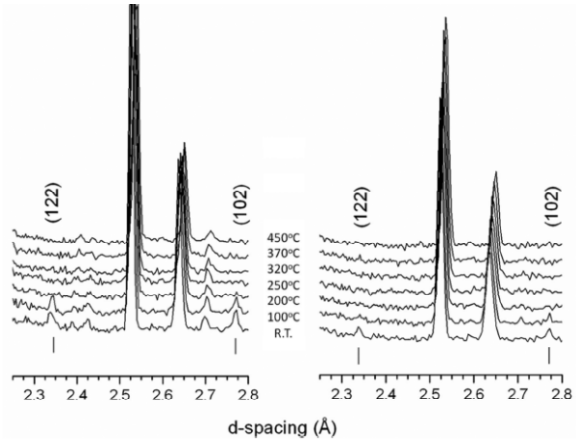

Figure 1: Variable temperature powder neutron diffractograms collected on C2 at CNBC. The peaks are labeled with respect to space group *Pnma*. Left: $BaCe_{0.9}In_{0.1}O_3$ Right: $BaCe_{0.8}In_{0.2}O_3$

References

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[2] Knight, K. S. *Solid State Ionics* 2001, 145, 275−294.
[3] Lussier, J.A., Shafi, S.P., Donaberger, R.L.; Bieringer, M., *Inorganic Chemistry*, 2014, **53**, 8809–8815