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Chemical expansion and proton conductivity in vanadium-substituted variants of $\text{-Ba}_4\text{Nb}_2\text{O}_9$

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Complex perovskite derived oxides are an important emerging class of ionic conducting materials with potential applications in energy technologies including fuel cells, batteries, and separation membranes. The high temperature phase $\text{-Ba}_4\text{Nb}_2\text{O}_9$ is one such complex oxide which shows proton and oxide ionic conduction.

Recently we have shown that two new compositional series with the previously unique $\text{-Ba}_4\text{Nb}_2\text{O}_9$ type structure, $\text{-Ba}_4\text{V}_x\text{Ta}_{2-x}\text{O}_9$ and $\text{-Ba}_4\text{V}_x\text{Nb}_{2-x}\text{O}_9$ ($x = 0-2/3$), can form [1]. Undoped $\text{Ba}_4\text{Ta}_2\text{O}_9$ forms a 6H-perovskite type phase, but with sufficient V doping the -type phase is thermodynamically preferred and possibly more stable than $\text{-Ba}_4\text{Nb}_2\text{O}_9$, forming at a 200 °C lower synthesis temperature. This is explained by the fact that Nb^{5+} ions in $\text{-Ba}_4\text{Nb}_2\text{O}_9$ simultaneously occupy 4-, 5- and 6-coordinate sites in the oxide sublattice, which is less stable than allowing smaller V^{5+} to occupy the former and larger Ta^{5+} to occupy the latter. We characterised the structures of the new phases using a combination of X-ray and neutron powder diffraction. All compositions hydrate rapidly and extensively (up to 1/3 H_2O per formula unit) under ambient conditions, like the parent $\text{-Ba}_4\text{Nb}_2\text{O}_9$ phase, and show moderate but improved mixed-ionic electronic conduction. At lower temperatures the ionic conduction is significantly protonic, where hydration is maintained. We also show that these new vanadium containing phases have higher total conductivities than the parent $\text{-Ba}_4\text{Nb}_2\text{O}_9$ compound.

[1] AJ Brown, B Schwaighofer, M Avdeev, B Johannessen, IR Evans and CD Ling, Chemistry of Materials, available online (2021). DOI: 10.1021/acs.chemmater.1c02340

Presenter Gender

Man

Do you wish to take part in the Student Poster Slam

No

Condition of submission

Yes

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Yes

Level of Expertise

Student

Pronouns

He/Him

Which facility did you use for your research

Australian Centre for Neutron Scattering

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