Local structures in BIMEVOX oxide ion conductors

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Keywords: local structure, total scattering, solid electrolyte

Despite concern over their stability in reducing atmospheres, the use of bismuth oxide based solid electrolytes in solid oxide fuel cells has recently been demonstrated as feasible [1]. The best low temperature oxide ion conductors known are the BIMEVOX (Bi2Mei,Vl/2O5.5−(5−l)/2, Me = dopants, l = valency) family of solid electrolytes based on substitution of V and or Bi in Bi4V2O11−δ [2]. A huge variety of cations have been successfully used as substituents to stabilize the disordered γ-phase to low temperature, most notably divalent cations such as Cu2+(x = 0.10) with conductivity of ca. 10−3 S cm−1 at 237 °C [2]. The high conductivity is affected by local structures, including preferred coordination, atom distribution and defect ordering. However, details of local structure are difficult to access and have rarely been reported.

In past, examination of local structure in BIMEVOXes relies mostly on careful analysis for the average structure using neutron/X-ray diffraction and Rietveld refinement [3,4]. The development of total scattering methods in recent years has afforded the opportunity of re-examining the local structure of the BIMEVOXes and the parent compound Bi4V2O11−δ in ways that were not previously possible, to yield a better understanding of the structure-conductivity relationship in these important systems. We have recently reported the local structure analysis for tetravalent- and trivalent-substitution BIMEVOX (ME = Ge, Ga) systems, and found special vacancy deficiency ordering in the former case [5, 6]. Therefore, in the current work, we focus on Bi2V0.9Cu0.1O5.35 and its parent compound Bi4V2O11−δ, using neutron total scattering technique plus the Reverse Monte Carlo (RMC) simulation methods, to detect their local structure and possible structure-property relationships. New findings in this type of complicated oxide ion conductors will be presented on the conference.


Fig. 1 Ideal structure of γ-BIMEVOX and positions of apical and equatorial vacancies.

Fig. 2 Fitted pair distribution function of Bi2V0.9Cu0.1O5.35 using RMC calculation.