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Structure of NaREPSiO (RE = Sc, Y) Glass-Ceramics probed by Solid-State NMR

I.D.A. Silva,[1]; A.M. Nieto-Munoz[2]; A.C.M. Rodrigues[2]; H. Eckert[1,3]
[1]São Carlos Institute of Physics, USP, São Carlos, Brazil
[2]Laboratory of Vitreous Materials, DEMa, UFSCar, São Carlos, Brazil
[3]Institut für Physicalische Chemie, WWU, Müster, Germany
e-mail: i.danciaes@gmail.com

The design of Na-ion all-solid-state batteries requires the optimization of materials to be used as solid electrolytes. Fast ion-conducting glass-ceramics are suitable for this purpose since they present the features of both glass phase and fast ion-conducting crystallites[1]. Glass-ceramics based on superionic crystalline $Na_5RESi_4O_{12}$ (N5, RE = Sc, Y) can be produced by controlled crystallization of sodium silicate glasses with specific compositions [2] and can reach ionic conductivities up to 0.1 S/cm [3]. Their compositions and properties can be isostructurally modified by Si –> P substitution. Precursor glasses of compositions $Na_{3.9}RE_{0.6}P_{0.3}Si_{2.7}O_9$ (NREPS) and $Na_{4.2}RE_{0.6}Si_3O_9$ (NRES), (RE = Sc, Y), were synthesized by the melting-quenching technique, and glass-ceramics were prepared according to the crystallization temperatures found by DSC. X-ray diffraction pattern of the glass-ceramics showed that the N5 crystal structure was found for NScS and NScPS glass-ceramics annealed at 905 and 925 °C, respectively. Multinuclear (^{29}Si, ^{23}Na, ^{31}P and ^{45}Sc) MAS NMR was used to monitor the conversion of the glassy precursor phase into the multi-phase glass ceramics at different stages of thermal annealing, confirming the successful substitution of $(SiO_4)^{4-}$ by $(PO_4)^{3-}$ ions in the N5 structure.

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