

Influence of lattice defects on the high pressure elastic properties of $\text{Ni}_{0.66}\text{Mn}_{2.33}\text{O}_4$ NTC materials

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Tuneable chemical compositions and cation displacement in spinel oxides offer great possibilities for manipulating physical and chemical properties of $\text{Ni}_x\text{Mn}_{3-x}\text{O}_4$ oxides. Owing to its negative temperature coefficient of resistance (NTC), NiMn_2O_4 is used for devising temperature sensors. The properties and hence the applications of $\text{Ni}_x\text{Mn}_{3-x}\text{O}_4$ oxide strongly depend on the Ni:Mn ratio, valence states, defects and cation distribution in the spinel structure. Many advantages of nickel-manganese oxide of the spinel structure as the cathode material have been also demonstrated in rechargeable aqueous zinc-ion batteries. Its electrochemical properties can be improved by controlling the molar ratio of Ni and Mn at the spinel cationic sites.

Here, the accuracy of determination of nickel and manganese cations distribution in the spinel structure of $\text{Ni}_{0.66}\text{Mn}_{2.34}\text{O}_4$ oxide, has been improved by taking into account the presence of tetrahedral vacancies. Additionally, the structural stability of cubic $\text{Ni}_{0.66}\text{Mn}_{2.34}\text{O}_4$ was investigated as a function of pressure up to 9.5 GPa using synchrotron radiation angle-dispersive X-ray powder diffraction and a diamond anvil cell. The bulk modulus and its first derivative were determined by fitting the Birch-Murnaghan equation of state (EoS) model to the experimental pressure-volume data. Rietveld refinement of the X-ray powder diffraction data reveals that the cubic spinel structure is stable upon compression to 9.5 GPa. The obtained data were discussed in terms of defects in the cationic sublattice and compared with the elastic parameters of NiMn_2O_4 [2].

[1] Uppuluri, K., and Szwagierczak, D.: Fabrication and characterization of screen printed NiMn_2O_4 spinel based thermistors. *Sensor Rev.*, 42(2), 177-186 (2022).

[2] Darul, J., and Piszora, P.: Influence of lattice defects on the high pressure properties of $\text{Ni}_{0.66}\text{Mn}_{2.33}\text{O}_4$ NTC ceramics. *Ceram. Int.*, 49(6), 9412-9418 (2023).

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