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Cadmium doping in vanadium oxides and Cadmium vanadates investigated by hyperfine interactions at ^{111m}Cd probe nuclei

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Vanadium oxides and vanadates are nowadays the best candidates for the next generation of battery cathode for energy storage,[1,2] particularly for the aqueous zinc-ion bateries (AZIB) due the low cost and good diffusion of Zn [3]. Hydrated vanadium pentoxide ($V_2O_5 \cdot nH_2O$) has
a bilayer structure and structural water molecules work as pillars to expand the layer spacing, and the shielding effect from water hinders the electrostatic interaction between cations accelerating the Zn ion diffusion. The doping with impurity cations (such as Mn, Al, and Zn) into the interlayers can improve the (de)intercalation of Zn ions by enlarging the spacing and obtaining a faster ion diffusion. Cd ion is 24% larger than Zn and, therefore, can help form a more efficient cathode.

In the work here reported, electric quadrupole interaction on ^{111m}Cd nuclei implanted in divanadium pentoxide doped with different concentrations of Cd were measured with time-differential perturbed angular correlations (TDPAC). Pure V_2O_5 as well as doped with 1%, 5%, and 10% of Cd were measured at different temperatures. Samples of the vanadates CdV_2O_6 and $Cd_2V_2O_7$ were also investigated. The intention is to provide a comprehensive description of the doping effects on the local crystal structure and the electronic structure around the impurity and the consequences on the properties of the host oxides. Results show that the probability of formation of cadmium vanadates is low but the temperature and atmosphere of measurements have an important effect at the local scale. Moreover, the temperature behavior of the hyperfine parameters of pure and Cd-doped V_2O_5 are similar to but distinguishable from the cadmium vanadates.

References

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