Poster Presentation

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Anisotropic strain and Jahn-Teller effect of chiral complexes and metal oxides

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For about a decade, we have systematically investigated thermally-accessible lattice strain and local pseudo Jahn-Teller distortion of [CuL2]3[M(CN)6]2•4H2O (L = (1R, 2R)-cyclohexanediamine; M = Cr, Co, and Fe). In mononuclear Cu(II) complexes, (pseudo) Jahn-Teller effect plays an important role in flexible distortion of crystal structures especially Cu(II) coordination environment. Beside Jahn-Teller distortion, we have dealt with some factors for example, metal substitution as bimetallic assemblies, chirality of ligands, and H/D isotope effect to vary intermolecular interaction and crystal packing. According to the course work using variable temperature PXRD, we have found that anisotropy of crystal strain distortion did not corporate with Jahn-Teller distortion around local coordination environment because of the discrepancy of the crystallographic axes and molecular alignment. In order to elucidate the anisotropic control of lattice strain and Jahn-Teller distortion closely, we have employed transition metal oxide with orthogonal or layered structures to prepare composite materials with the chiral metal complexes for discussion of thermally-accessible PXRD changes and IR shift due to adsorption. At first, we have employed chiral one-dimensional zig-zag Cu-Cr bimetallic assemblies and their oxides prepared by burining. Based on variable temperature XRD patterns, a linear correlation (lnK = a/T + b) of K (=d(T)-d(0)/d(T)) values, where d(T) and d(0) are spacing of lattice plane (d = nl/(2sinq)) at T K and 0 K (extrapolated), respectively, and its deviation from ideal correlation indicates degree of anisotropic lattice distortion of the composite materials. For example, we could observe LiMnO2, typical material of lithium ion battery, was enhanced anisotropic lattice strain along the b axis or the (011) plane added by [CuL2(H2O)2](NO3)2 complexes. Which may prevent from breaking down regular crystal structures during charge-discharge of secondary battery.

[1] *D. Tazaki, Y. Orii, & T. Akitsu, Cobalt : Characteristics, Compounds and Applications, Nova Science Publishers, Inc. (NY, USA), chapter 13, 315 (2013).*

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