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Structural evolution of Tungsten Oxide Network during WO3.H2O formation

Content

Tungsten Oxides (WO_x) are well known for their versatile structures and properties (photo and electrocatalysis, electrochromism, energy storage…), often enhanced at nano-scale, leading to broad applications (smart windows, pollutant degradation…). [1-2] Tungsten Hydrate $WO_3 \cdot H_2O$ is here prepared at room temperature using sol-gel synthesis: The initial Decatungstate $W_{10}O_{32}$4- evolves to amorphous gels, and within few days, toward crystalline $WO_3 \cdot H_2O$ powder. [3]

We focus on the pathway from corner and edge sharing WO_6 octahedra $W_{10}O_{32}$4- clusters to only corner sharing WO_6 octahedra $WO_3 \cdot H_2O$ structure, using X-ray Total scattering diffusion coupled to Pair Distribution Function analysis (ID11, ESRF).

PDF curves show short range organization for the amorphous gels. A Machine Learning-Motif Extractor (ML-MotEx) [4] code was used to determine the structural features of the 2h gel. Indeed, this code allows to extract, from a given model, the atoms contributing positively or negatively on the fit results. For the 24h gel, a clusters approach has enabled us to propose a checkerboard finite features that can be seen as early nucleation of the final hydrate WO_3 structure.

PDF refinement on the final powder clearly shows that the use of the usual crystalline Pnmb $WO_3 \cdot H_2O$ structure on the entire distance range (1.4–60Å) is not sufficient. Implementing sequential fit in r series has led to the description of two zones: Short Range Order (SRO) for 1.4-20 Å, and Long Range Order for 20– 60Å. Separate refinements, as it has been proposed by Juelsholt et al. [5], show a distorted P1 SRO structure whereas it remain close to the published Pnmb $WO_3 \cdot H_2O$ for LRO.

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[4] A. S. Anker et al. npj Comput. Mater. 8, 213 (2022) https://doi.org/10.1038/s41524-022-00896-3
[5] M. Juelsholt et al.J. Phys. Chem. C, 123, 5110 (2019) https://doi.org/10.1021/acs.jpcc.8b12395

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