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Study of the Properties of Commercial Nb_2O_5, Under Thermal Treatment

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Highlights

Calcination under high temperatures increases material crystallinity, while specific surface area decreases.

Materials treated in oven, above 800 °C had residue 78.6%w/w, compatible with $Nb_2O_5 \cdot 4H_2O$.

Abstract

Niobium pentoxide (Nb_2O_5) is a semiconductor (bandgap ~3,4 eV) commonly applied to photocatalysis and electrical devices. Its properties can change according to the synthesis method and crystallographic phase. Four stable phases of Nb_2O_5 are related in the literature [1]: monoclinic (H), tetragonal (M), orthorhombic (T) and pseudo-hexagonal (TT). This work investigates the calcination of commercial Nb_2O_5, HY-340[2], in air atmosphere, and studies the effect of thermal treatment (at 110, 200, 350, 600, 800 and 1000 °C, for 20 h). Figure 1 shows two steps of mass loss, 70.4 °C corresponding to adsorbed water, and 120.1 °C corresponding to bound water. Above 337.2 °C the material becomes thermally stable leaving an 86.0% residue. Calcination residues in a muffle furnace ranged from 86.2 to 78,6% w/w, consistent with $Nb_2O_5 \cdot 2.5H_2O$ and $Nb_2O_5 \cdot 4H_2O$ stoichiometries. XRD analysis showed that the material remains amorphous up to 350 ºC. At 600 °C a pseudo-hexagonal phase mixed with orthorhombic is observed. At 800 °C, only orthorhombic phase is present and at 1000 °C, the material is converted to monoclinic phase. Crystallite size determined by Scherrer's equation ranged from 60.1 to 134.1 nm. Specific surface area (SSA) decreased from 6.8 to 0.1 $m^2\ g^{-1}$ for crystalline material, which is not significant due to instrumental technical errors. For amorphous material, SSA ranged from 171.3 to 108. 7 $m^2\ g^{-1}$, making them suitable for catalytic applications, as adsorption studies indicated type IV isotherms[3].

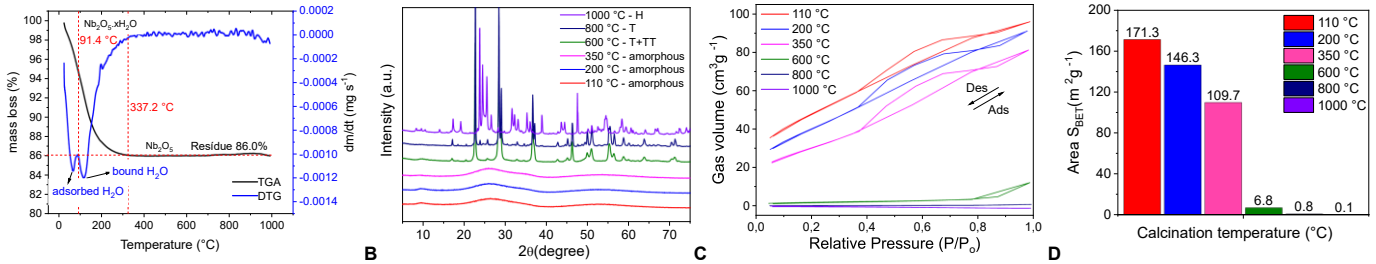

Figure 1 – A) TGA/DTG (TA Instruments Q20®, sample HY-340 in synthetic air, 10 °C min^{-1}); B) XRD (Bruker D2 Phaser®, 40 kV, 15 mA, 1º min^{-1}, CuKα (λ = 1,5418 Å); C) Isotherms of N_2 77 K, (Quantachrome 2200 NovaWin®); D) Specific surface area SSA - S_{BET} multipoint, 20 pt.

References

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