Structural and morphological properties of ultrasonic-modified $NiMoO_4$ hydrate

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Introduction

Nickel molybdate ($NiMoO_4$) with its low cost, safe use, and improved electrochemical performance, is a potential candidate for applications in energy storage devices, namely hybrid capacitors. To improve the specific capacitance, power and energy of hybrid capacitors, various methods of cathode material modification are used. Ultrasonic modification is a promising method of controlled change in the particle size and the surface area of nanomaterials.

Methods

We analyzed the crystal structure and morphology of nickel molybdate hydrate obtained by hydrothermal method [1] and modified by ultrasound (the operating frequency is 22 kHz) for 15, 60 and 90 minutes. The crystal structure was investigated by powder X-ray diffraction analysis using a diffractometer DRON (Cu-Kα radiation, wavelength 0.15405 nm). The morphological properties were investigated by the low-temperature nitrogen absorption / desorption porosimetry (Quantachrome Autosorb Nova 2200e device).

Results

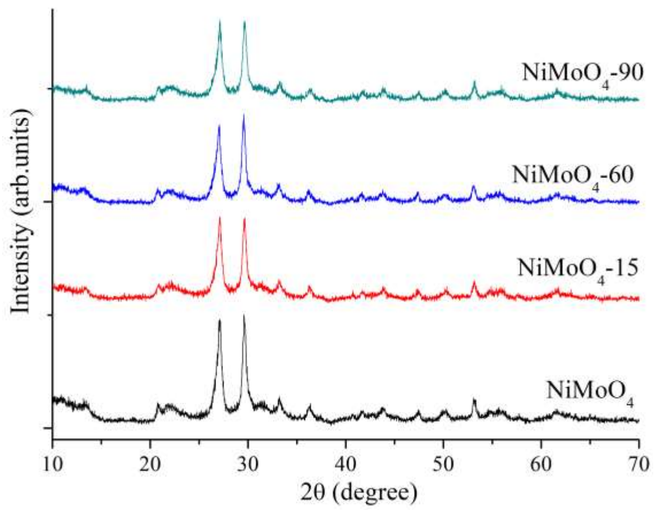

Figure 1. X-ray diffraction patterns

- The average crystallites size, calculated by the Scherrer equation, was 17 nm for the initial nickel molybdate and for all modified samples.

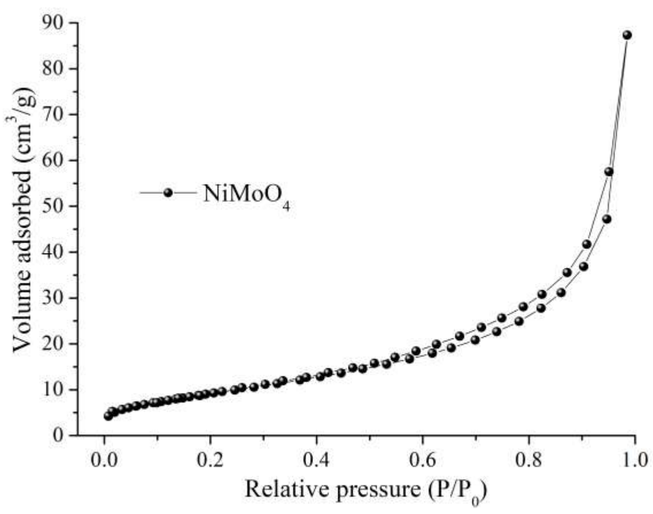

Figure 2. Nitrogen adsorption-desorption isotherms (−196 °C)

- IV hysteresis is observed for all materials (according to UIPAC classification [2]) in the range P/P_0 0.5–1.0. The specific surface area of the initial nickel molybdate was 31 m^2/g and does not change for the modified materials (28-31 m^2/g).

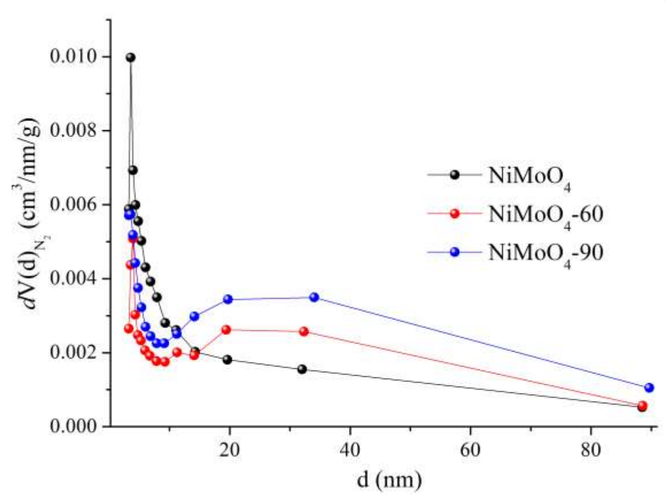

Figure 3. BJH pore size distributions plots

- The pore size distribution spectra determined by the Barrett – Joyner – Halenda method indicate the mesoporous structure of nickel molybdates and an increase in the average pore diameter from 17 nm for the initial nickel molybdate to 28.8 nm for material modified by ultrasound for 90 min.

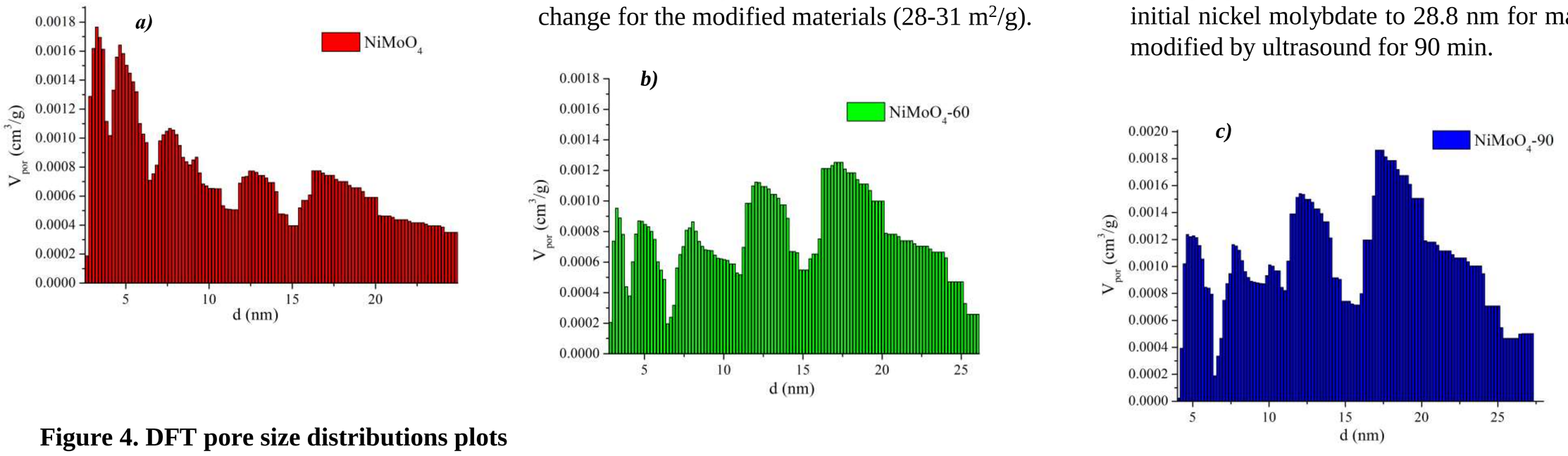

Figure 4. DFT pore size distributions plots

- DFT histograms indicate a wide pore size distribution in the range of 2-26 nm and an increase in total mesopores volume from 0.135 cm^3/g to 0.223 cm^3/g with prolonged ultrasonic dispersion.

Conclusion

Thus, ultrasonic modification does not change the crystallite size of $NiMoO_4$ hydrate, however, in modified materials there is a redistribution of pores in size, namely, the volume of mesopores with a diameter of 20-28 nm increases. This is due to the fact that at ultrasonic frequencies from 20 kHz to 50 kHz, the most common are physical effects, including shock waves, which accelerate solid particles suspended in the liquid, causing changes in the morphology of materials.

References

1. Popovych, O. M., Budzulyak, I. M., Yukhymchuk, V. O., Budzulyak, S. I., & Popovych, D. I. (2021). Raman spectroscopy of nickel molybdate and its modifications. Fullerenes, Nanotubes and Carbon Nanostructures, 29(12), 1009-1015.
2. Thommes, M., Kaneko, K., Neimark, A. V., Olivier, J. P., Rodriguez-Reinoso, F., Rouquerol, J., & Sing, K. S. (2015). Physisorption of gases, with special reference to the evaluation of surface area and pore size distribution (IUPAC Technical Report). Pure and applied chemistry, 87(9-10), 1051-1069.