The role of the crystallographic orientation of the oxide materialsin their gas sensing activity

N.E. Boboriko
Chemistry Faculty, Belarusian State University, Minsk, Belarus,
e-mail: *boboriko@bsu.by*

One of the tools to evaluate gas sensing properties of the oxide materials with a minimal empirical experimental search is molecular dynamics simulation [1]. It allows analyzing the interaction of the detecting molecule with the surface of gas sensing material and revealing the most energy-efficient contacts. The ability of the oxide surface to interact with the molecules of the detecting gas is essential in the forming of gas sensing properties.

It is obvious that the process of adsorption of the gas molecules at thermodynamically unstable oxide surfaces is more efficient in comparison with the adsorption at thermodynamically stable ones. The same statement comes from the analysis of the results of the molecular dynamics simulation of the interaction of CH_4, H_2, C_2H_5OH, and H_2O molecules with TiO_2 and MoO_3 atomic planes of {100} set [1]. The problem is that the existence of thermodynamically unstable planes in a large quantity in a real oxide material is unprofitable and highly improbable. This opens a problematic area of the aimed synthesis of the crystallographically oriented oxide materials.

In the work MoO_3 with the pronounced (010) orientation was synthesized by a simple and fast route by the heat treatment of the mixture of $(NH_4)_6Mo_7O_{24}\cdot 4H_2O$, oxalic acid, and Pluronic F-127 at 450 °C for 4 hours.

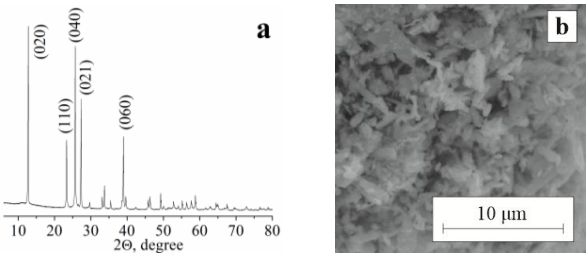

Fig. XRD pattern (a) and SEM image (b) of the oriented MoO_3

Molecular dynamics simulation showed that MoO_3 (010) atomic planes are perspective for the interaction with C_2H_5OH molecules. It was established that the output value towards ethanol of the semiconducting chemical gas sensors on the basis of "TiO_2 - oriented MoO_3" material is about 20 % higher than of the sensors based on "TiO_2 - spherical MoO_3", obtained by the calcination of $(NH_4)_6Mo_7O_{24}\cdot 4H_2O$ at 450 °C.

Reference

[1] N.E. Boboriko, Y.U. Dzichenka. J. Alloy. Compd. (2021) 855: 157490.