Gas Sensing with Nanocrystalline Tetragonal WO_3 Films

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Abstract

A high-temperature route employing advanced reactive gas deposition was used to produce WO_3 nanoparticles with the metastable tetragonal crystal structure for gas-sensing applications. WO_3 thick films of the produced nanoparticles were deposited on alumina substrates with pre-printed gold electrodes, being 200 μm apart, and a Pt heating resistor printed on the reverse side. WO_3 is an extrinsic n-type semiconductor and its crystal structure is lowered from the ideal cubic symmetry of the metallic ReO_3 and isoelectronic $NaWO_3$ bronze. The oxygen octahedra in WO_3 are deformed and tilted and the metal cation lies off-center. Because of this great flexibility inherent in the structure, there are many different types of distortions (phases) at different temperatures and the physical properties of the structures depend crucially on the details of these distortions. The high-temperature tetragonal phase of WO_3 has a layered structure perpendicular to the tetragonal c axis, which implies a stable (001) surface for tetragonal crystallites. This layered crystal structure is interesting from the point of gas sensing, since it contains terminal-like W = 0 bonds on both sides of each layer through the structure, in addition to surfaces, and also large 12-fold coordinated cages for ion insertion into the structure.

The WO_3 films were very sensitive, e.g., to H_2S already at room temperature and to NO_2 at low temperatures above about 450 K. Maximum sensitivity in synthetic air to H_2S was found at about 400 K and to NO_2 at about 525 K. Gas sensitivity was studied also in atmospheres having different oxygen concentrations. E.g., the temperature corresponding to the maximum sensitivity to H_2S was found to increase with decreasing oxygen concentration in the atmosphere.