Nanostructured surfaces

EFFECT OF DEVIATIONS FROM STOIHOMETRIA ON ELECTROSTATIC POTENTIAL OF SURFACE OF VANADIUM DIOXIDE

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The phase transition of «insulator-metal» in vanadium dioxide takes place at 338–340 K, accompanied by hopping changes in optical and electric properties of the substance. For vanadium oxides it is peculiar to form as Magneli phase with change of symmetry of structure, and defective structures (where it is little bit more than atoms of oxygen or less norm) with preservation of symmetry of the basic phase of oxide of metal. In the presented work calculations of electrostatic potential of a surface of "flat" models of a surface VO_2 which contain 10 and 16 formular units are carried out. The calculations were carried out by Hartree-Fock-Roothaan method with basis set “mini” and” sbkjc” by means of the program package PC GAMESS and Firefly8.11 [1].

The structure of models after optimisation corresponds to structure of a semi-conductor phase with altered vanadium-vanadium intrteratomic distances (fig.1). Dark colour notes atoms of vanadium

1	2	3	4	5

Fig.1. Models of VO_2: 1-$16VO_2(14H_2O)$; 2-$10VO_2(12H_2O)$; 3-$10VO_{1.8}(8H_2O)$; 4-$10VO_{1.9}(7H_2O)$; 5-$10VO_{2.1}(5H_2O)$.

Distribution of electrostatic potential counted in a zone of influence of two central atoms of vanadium on surfaces. These atoms have absolutely identical coordination environment in all models. Maps of electrostatic potential slightly differ at basis use “mini” and” sbkjc” The received maps of electrostatic potential for models testify that intensity of field influence on environment molecules (for example, on water molecules) increases with increase in quantity of atoms of oxygen in model.

1. *Schmidt M.W., Baldridge K.K., Boatz J.A. et al. General atomic and molecular electronic structure system //* J. Comput. Chem.-1993.- **14**.- P. 1347.