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COMPUTER MODELING OF METAL OXIDES IN VESTA

Recently, computer modeling of solids is gaining popularity due to its possibilities to work simultaneously with both structural models and volumetric data, such as atomic and electron density, and comprehension of the experimental data obtained in three dimensions.

Among solid inorganic substances, nanodispersed oxides of materials have great popularity. Their use covers almost all areas of materials science, catalysis, sorption processes, sensorics, and many others [1].

In this paper the structures of titanium (IV) (anatase modification) and tin (IV) oxides are studied. They are widely used as sensitive layers of gas sensors, photocatalysts and sorbents [2]. Thus, modeling their structures would be for great interest for subsequent study and comparison of their electrical, sorption, catalytic and optical properties.

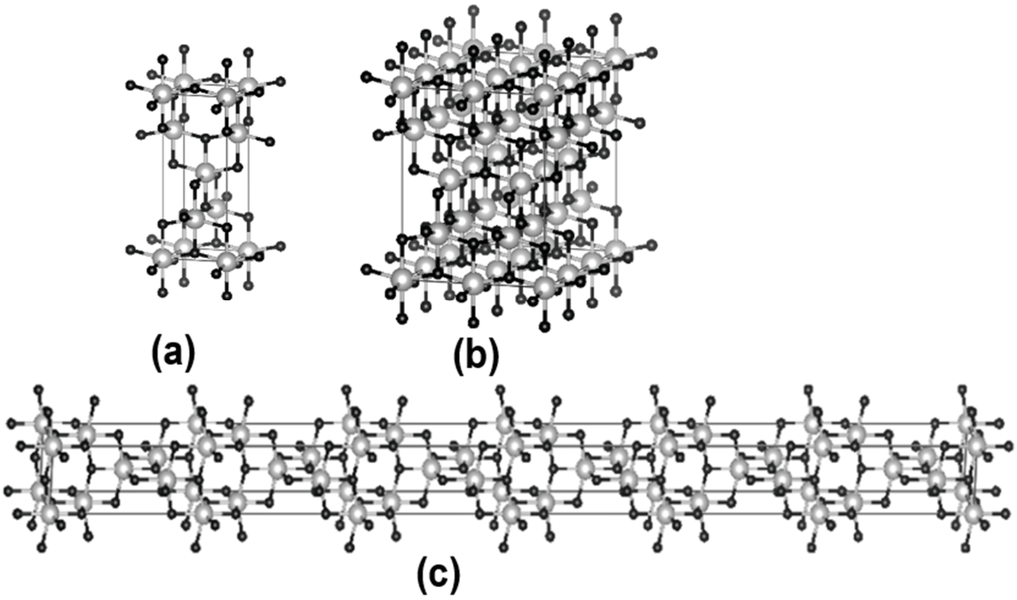

Figure 1 – Unit cells of titanium oxide (IV):
(a) – cell 1×1, (b) – cell 2×3, (c) – cell 6×1.

For modeling structures, programs such as ChemDoodle, Hypercube, Avogadro, BIOVIA Draw, VESTA (Three-Dimensional Visualization System for Electronic and Structural Analysis) are used, among which the latter has a number of positive characteristics. VESTA can deal with a virtually unlimited number of objects, such as atoms, bonds, polygons on isosurfaces, supports transformation of an convention elementary cell to non-conventional one using a matrix, visualizes interatomic distances and angles between bonds, calculates electronic and nuclear densities using the structure of compounds, has the ability to import files from similar programs. In addition, the important advantages of this program are its free distribution and the possibility of its use on the most common operating systems Windows, Mac OS X and Linux [3].

The modelling of elementary cells of titanium (IV) (anatase modification) and tin (IV) oxides was performed and results are depicted on Figures 1 and 2, respectively. The parameters of the unit cells for construction were taken from [4] and [5] for titanium oxide (IV) and tin (IV), respectively.

As seen, the program allows one to build not only the unit cell, but also add them together and represent different nanostructures, such as 0D, 1D, and even, if necessary, 2D nanostructures. At the same time, a file is created with the coordinates of each atom, which can be easily transferred to other programs, such as Chem3D, VASP etc.

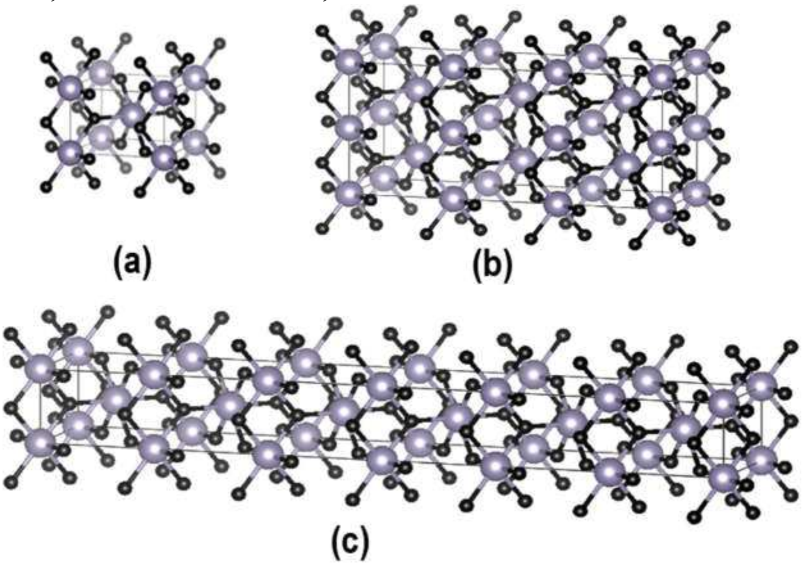

Figure 2 – Unit cells of tin oxide (IV):
(a) – cell 1×1, (b) – cell 3×2, (c)– cell 6×1.

Modeling the structure of metal oxides in this program will further facilitate the detailed study of the theoretical properties of these oxides, such as geometric optimization, the total energy of the system, and the energy of crystal faces.

LITERATURE

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SULFUR-CONTAINING BIOCARBON MATERIAL FOR STRONG BINDING OF HEAVY METALS

Pollution of soils with heavy metals (HM) is an important ecological problem. Removing heavy metals is a difficult task, since they often have a low concentration [1-3]. Heavy metals have the ability to various chemical and physico-chemical reactions. HM have the ability to move, to redistribute and to migrate. Various methods are used for ecosystems purification from heavy metals, including sorption. If we consider methods for cleaning contaminated soil, it is advisable to use the most ecological and safe methods for soil purification. It is possible to precipitate them in the form of sparingly soluble sediments, to wash them out of the soil profile, to extract from the soil by plants and microorganisms, to apply sorption by minerals with high cation exchange capacity and a mixture of sorbents. The disadvantages of the existing methods of cleaning soil from HM determine the need to find new methods of soil detoxification.

Elimination of the mobility of heavy metals on the site has a lot of advantages over the physical removal. One way to stabilize heavy metals is to add chemicals to the soil that cause the formation of minerals containing