Popular Science project description

This project will study properties of metal oxides, relating to presence of point defects at moderate temperatures (below half of the melting point temperature, named as Tammann's temperature). Metal oxide exhibit the crystalline structure in which atoms or ions take place in the nodes of the crystal lattice of the one of the 230 space groups. However, the ideal ordered do not exist, practically. In the real crystals several types of defect exist. The defect can be in the valence electrons distribution (such defects are named as electronic defects) as well as in the distribution of atoms or ions, termed as atomic or ionic defects. There are two main sources of their formation: thermal vibrations of the crystal lattice and frequently existing in metal oxides departure from the Proust's law (or the law of definite composition) named also as departure from stoichiometry.

Usually, defected solid is treated as solid solution, in which the crystal lattice is a 'solvent' and point defects are solutes. If concentration of the solute below 0.1 at.% the solution can be treated as ideal. It results from the assumption negligible low interactions between defects. In this case the equilibrium constant of the defect reactions (termed as quasi-chemical reactions) may be expressed by the concentration of defects instead of their activities. The assumption of the lack interactions is rather valid at high temperatures. It is close analogy with gas systems. Gases at high temperature and low pressure obey laws of the ideal gases, because the interaction between gas molecules is negligible. But, when gas is quenched and compressed , then interaction between molecules plays important role and as a result gas undergoes condensation.

Analogously, at lower temperatures interaction between defects cannot be omitted. Then, point defects instead their randomly distribution in the crystal lattice form agglomeration such as complexes, clusters, shear planes or incipient of new phase. Moreover, during quenching of the crystal the phenomenon the freezing of the defect reactions takes place.

Applying the ideal solution model to defected metal oxides at high temperatures, the theory has been obtained. This theory remains in good agreement with experimental results. Unfortunately, there are not similar theory in case lower temperatures. The purpose of this project is to fill this gap. To oxide systems were chosen in the work plan of the project: TiO_2 as a model , representing electronic semiconductor and solid solution of the yttrium oxide in zirconium dioxide: $(Zr_{1-z}Y_z)O_{2..x\ as\ a}$ model, representing ionic conductor.

Returning to the mentioned above gas system. Such system is characterizing of two features: concentration of the gas molecules and their mobility. Similarly, in this project both mentioned features will be studied:

- concentration of defects by means of the dete5rmination of nonstoichiometry, electrical conductivity, thermopower, and
- mobility by determination of the diffusion coefficients.

Both cases will be discussed: model of ideal point defect and model of the point defects where interaction will be taken into account.