

Nanostructural engineering of oxide ceramic materials

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Physical properties of ceramic materials are strongly influenced by the inherent properties of the bulk crystalline material, by grain boundary effects and the effects caused by a presence of fault structures. Out of these, special grain boundaries appear to be of the top importance from both microstructural and the compositional point of view. As recently shown in several polycrystalline materials, special boundaries are responsible for anisotropic and exaggerated grain growth. The influence of these defects on the microstructure of the ceramic and consequently to the physical properties is thus commonly observed, and yet the knowledge on their formation mechanisms or the atomistic structure and chemistry has not evolved. One of the main reasons is the availability of the instrumentation that allows the atomic level studies of structure and composition of special boundaries and interfaces, combined with an appropriate expertise in materials science. In order to determine a mechanism of their formation one must commence not only with the information on the preparation conditions under which such a phenomenon takes place, but moreover with a basic knowledge about their local structure and chemistry.

In semiconducting materials, such as ZnO, GaN and AlN, among others, special boundaries play the key role in crystal growth, and modify the physical properties of the crystals or crystalline films, having far reaching implications on the electronic and optical properties of devices based on these materials. The proposed research fits in the field of local phase transformations on the atomistic scale in relation to the microstructural properties of semiconducting materials. The most common type of sub-nanometer special boundaries in semiconducting materials are the so-called inversion boundaries that form in noncentrosymmetric crystals, such as ZnO, GaN and AlN, by the addition of specific dopants. The major task within of our research is to correlate the atomistic structure and chemistry of special boundaries with the exaggerated grain growth and the final physical properties of the material. Such a bottom-up approach provides the means for nanostructural engineering of various electronic devices based on these materials.