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Computational materials science aided design of glass ceramics and crystal properties

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Abstract

Today's high tech materials have in many cases highly specialized properties and designed functionalities. Materials parameters like high temperature stability, high stiffness and certain optical properties have to be optimized and in many cases an adaptation to given processes is necessary. Many materials are compounds or layered structures. Thus, surface and interface properties need to be considered as well. At the same time to some extent just a few atomic layers sometimes determine the properties of the material, as is well known in semiconductor and other thin film technologies. Therefore, a detailed understanding of the materials properties at the atomic scale becomes more and more important. In addition many high tech materials have to be of high purity or selective dopant concentrations have to be adjusted to fulfill the desired functionality. Modern materials developments successfully use computational materials science to achieve that goal. Improved software tools and continuously growing computational power allow us to predict macroscopic properties of materials on the basis of microscopic/atomic *ab initio* simulation approaches.

At Schott, special materials, in particular glasses and glass ceramics, are produced for a variety of applications. For a glass ceramic all the above mentioned difficulties for materials development arise. The properties of a glass ceramic are determined by the interplay of crystalline phases embedded in an amorphous glass matrix. For materials development the understanding of crystal structures and their properties, surfaces and interface phenomena, and amorphous systems are necessary, likewise. Each by itself is already a challenging problem. Many crystal phases that are grown within the glass matrix do not exist as single crystals or are difficult to grow in reasonable amounts for experimental investigations. The only way to obtain the properties of these crystalline phases is through '*ab initio*' simulations in the computer.

In this presentation results of density functional theory (DFT) calculations of various crystal structures, mainly oxides, are discussed. The focus is on the thermomechanical and optical properties. We present elastic properties and the anisotropic Young's modulus for spinel structures, pyrosilicates and further oxides like rutile. Their influence on the stiffness of a resulting glass ceramic is discussed. The thermal expansion of glass ceramics is an important feature and is strongly dependent on the coefficient of thermal expansion (CTE) of the crystalline phases. For selective oxides the calculation of the CTE in the harmonic approximation is presented and a comparison with experiments is given.

Optical devices for microlithography use CaF_2 crystal as a lens material. The optical properties and the influence of certain impurities in CaF_2 are crucial for the performance of such devices. '*Ab initio*' simulation helps us here to estimate the formation of defects and color centers. Local density approximation screened exchange calculations for the optical properties of CaF_2 are presented as well as DFT simulation results for impurities and defects.

