Ab initio modeling of materials with defects

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Crystal defects modify the basic physical and chemical properties of materials. This effect is enhanced in materials with tendency to accumulate a large number of native defects or due to irradiation. The accuracy of *ab initio* modeling, involving no experimental input parameters, is now sufficient for the meaningful analysis of materials properties. First principles calculations provide relevant information about the formation energies of defects, the structure of nanoscale defects and about the nature of short-range interactions between defects, clustering of defects, and their migration. A good example of a material with a large number of native defects is iron oxide $Fe_{1-x}O$ (wustite), which is an important component of the Earth's interior. A*b initio* studies based on the density functional theory (DFT) explained the strong influence of cation vacancies with natural concentration x~5-15% on the structural, electronic, and dynamical properties of wustite [1,2]. A number of problems in the development of nanoelectronics are tightly connected with the understanding of defects, usually associated with harmful effects on device operation (traping free carriers, reducing the carrier lifetime). But some properties such as the vacancy-induced magnetism can be enhanced in samples irradiated by neutrons. I will present some examples of first principles studies on defects in silicon carbide (SiC) [3], a promising material for high-voltage and high-frequency nanoelectronic devices as well as for fusion reactor systems.

The DFT calculations provide the means for evaluating the structure of radiation defects and basic characteristics such as the energy of interaction between radiation defects and impurities, activation energies characterizing reaction rates and dynamics of migration and clustering of radiation defects. Higher neutron fluxes and higher average neutron energies in fusion reactors give rise to new precesses like the transmutation production of gas atoms (He, H) that have severe consequences for materials [4]. It generates also fundamental questions, which can be addressed within the *ab initio* studies: diffusion of gas atoms in the crystal, their clustering and accumulating at vacancies, dislocations or grain boundaries, their influence on structural and elastic properties of materials. These examples confirm the general importance of basic studies on crystal defects by the *ab initio* methods.

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