Defect substitution energies in cubic barium titanate

Juan J. Meléndez-Martínez[1], Y. A. Zulueta[2], Y. Leyet[3]

[1] Department of Physics, University of Extremadura. Badajoz (Spain)
[2] Departamento de Física. Universidad de Oriente. Santiago de Cuba (Cuba)
[3] Instituto Federal de Educação Ciência e Tecnologia, Manaus (Brazil)

The interesting electrical properties of $BaTiO_3$, which is an electric insulator at room temperature, can be substantially changed by doping. Thus, doping donor impurities may yield semiconducting behavior at low concentrations (typically less than 0.5 at. %) or to improved resistance to dielectric breakdown at higher concentrations [1]. Doping has also been shown to modify the ferroelectric behavior of these ceramics under some conditions [2]. Several types of impurities may be accommodated at different sites in the $BaTiO_3$, and each substitution mode involves different energetics, structural modifications and changes in physical properties.

Some previous works have dealt with the defect structure of $BaTiO_3$ based ceramics [3-5]. Most of them are based in Molecular Dynamics (coupled with dipolar corrections for charged defects [6]), and have been able to give some insight into the favorable substitution modes under given conditions. However, *ab initio* calculations have been barely used to characterize defects in $BaTiO_3$ ceramics [7].

In this work, defect energetics and structure for several substitution modes in Fe-doped $BaTiO_3$ are studied by *ab initio* calculations performed by a DFT formalism within the Linear Density Approximation coupled with Hubbard-type corrections for strongly correlated electrons. The results are compared and critically analyzed in terms of literature data, and preliminary assessments about the physical behavior of these systems are made.

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Nanostructuring Bi$_2$Te$_3$: influence on the phonon thermal conductivity

Natalia Bedoya, Adham Hashibon, Christian Elsässer

Fraunhofer-IWM, Wohlerstr 11, D-79108 Freiburg, Germany.

The use of thermoelectric materials to recover energy waste in form of heat has been limited so far by the low energy conversion efficiency. Recently, however, a renewed interest in these materials has arisen. An enhancement in their performance has been obtained mainly by lowering the phonon thermal conductivity due to nanostructuring, resulting in size confinement effects of the phonons and interface scattering [1]. The understanding of the vibrational properties of these materials, hence, is a key element to design and tailor their thermoelectrical properties. Here we study, by means of non-equilibrium molecular-dynamics simulations, the effects of dimensionality on the phonon thermal transport in Bi$_2$Te$_3$, the best known thermoelectric material for room temperature applications. In a first stage we analyze the influence of point defects on the phonon thermal transport of bulk Bi$_2$Te$_3$. Four types of defects at different concentrations are considered namely Bi and Te vacancies and antisites. A reduction of up to 50% of the bulk thermal conductivity is obtained, with a weak dependence on the nature of the point defects. The picture of dimensionality is then completed by studying the geometry dependence of the thermal conductivity in Bi$_2$Te$_3$ nanowires. All our results are analyzed in terms of the vibrational properties, providing a detailed atomistic study of the phonon thermal transport in the systems considered.

A study of iron impurities interacting with grain boundaries in photovoltaic silicon using density functional theory

Benedikt Ziebarth[1,2], Matous Mrovec[1], Christian Elsässer[1], Peter Gumbsch[1,2]

[1]Fraunhofer-Institut für Werkstoffmechanik IWM, 79108 Freiburg, Germany
[2]Karlsruher Institut für Technologie, Institut für Angewandte Materialien (IAM-ZBS), Engelbert-Arnold-Str. 4, 76131 Karlsruhe, Germany

Iron impurities have a negative effect on the efficiency of silicon-based solar cells because they act as trapping centers for charge carriers. Different processing techniques are applied to improve the efficiency by passivation of the iron contamination. For instance, internal gettering exploits the attractive interaction between the preexisting grain boundaries and the diffusing iron atoms. Therefore, it is interesting and important to build up a fundamental understanding of this interaction mechanism. To this end density functional theory is used to study the segregation mechanism for the impurity atoms at grain boundaries. The set of investigated symmetrical tilt grain boundaries in Si provides a variety of interface orientations and structures at the atomic scale. While some of the grain boundaries show very large segregation energies for interstitial Fe, most of these Si grain boundaries repel single interstitial Fe. Occasionally we find some grain boundaries to favor collective segregation of multiple Fe atoms, which may indicate a potential formation of Fe-Si precipitates at grain boundaries.

Passivation of silicon surfaces by aluminum oxide layers: a simulation study

Francesco Colonna[1,2], Christian Elsässer[1,2]

[1] Freiburg Materials Research Center, University of Freiburg, Germany
[2] Fraunhofer Institute for Mechanics of Materials IWM, Freiburg, Germany

By the Atomic Layer Deposition of Aluminum Oxide on a Silicon (100) surface, followed by a heat-treatment, it is possible to obtain an excellent surface passivation [1], which has the potential to enhance the efficiency of energy conversion in photovoltaic applications.

For a thorough understanding of the passivation process it is necessary to elucidate the interplay between physical properties at the electronic and atomistic scale. To this end we model the Silicon-Alumina interface by means of ab initio density functional theory (DFT) methods. Following experimental observations, we investigate the relation between chemical passivation and the local tetrahedral and octahedral environments in the alumina phase. To this end we simulate a number of stoichiometric and oxygen-rich models of interface between Silicon and k-Alumina, which entails both tetrahedrons and octahedrons as local environments at the interface. We also study the role played by the amount of Hydrogen at the interface, which is known to change during the heat treatment [2]. To obtain an accurate description of defect states in the band gap we refine our electronic structure simulations by applying a state-of-the-art DFT self-interaction-correction.

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A hybrid quantum classical simulation on the diffusivity of Li's in the graphite

Shuji Ogata,[1] Nobuko Ohba,[2] Takahisa Kouno[3]

[1]Graduate School of Engineering, Nagoya Institute of Technology, Japan
[2]Toyota Central Research & Development Laboratories, Inc., Japan
[3]Institute for Solid State Physics, The University of Tokyo, Japan

The Li-graphite intercalation compound is put to practical use as the negative electrode of the Li-ion batteries (LIBs). The transport property of the Li-ion in the graphite is related to the output power of LIBs. We assumed the initial stage of the Li insertion into the graphite and applied the hybrid quantum (QM)-classical (CL) simulation for understandings of the thermal diffusion process of a single Li-ion in the graphite [1, 2]. In this study, the diffusion process of plural Li's in the graphite is analyzed with taking into account the interaction among the Li-ions.

In our hybrid QM-CL simulation, the number of atoms included in the QM-region is minimized within the physical accuracy tolerance, and the QM-region which consists of Li and the surrounding carbon atoms is selected adaptively following the migration of the Li-ion. The number of atoms (N) included in the QM-region increases in the case that plural Li's exist in graphite. Therefore the order-N type of divide-and-conquer-type real- space grid DFT code (DC-RGDFT) [3] is adopted for the QM calculation so as to reduce all calculation cost.

Firstly, seven Li's are placed near into the same layer of graphite. Then the Li's are scattered isotropically by the coulomb repulsion interaction. However, the expanse of the Li-ions is limited to the range of a radius of around 10 Å because of the cage effect. Figure 1 shows the distribution of the inter-layer distance (*d*) of the upper and lower graphite layers of Li's after 2.5ps hybrid simulation. The inter-layer distance of the graphite of the Li existing domain is longer than that of the domain where there is no Li, i.e., the cage effect is confirmed. An individual Li-ion diffuses well in the cage.
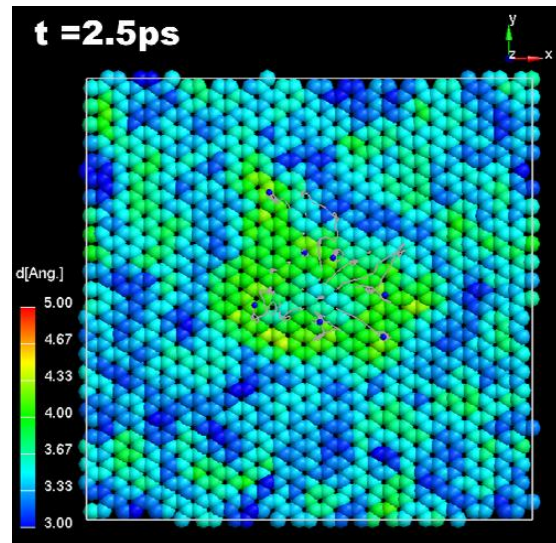

Figure1: The distribution of the inter-layer distance of the upper and lower graphite layers of Li's after 2.5ps hybrid simulation. The small blue spheres denote Li-ions, the grey lines shows the trajectories of Li's.

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