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Defect-Induced Effects in Nanomaterials

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A solid without defects is a utopia. The word was coined in 1516 from Ancient Greek (οὐ-τοπος) by Sir Thomas More for his Latin text *Utopia* and it means "no place". Perfect solids do not exist, much to the delight of the entire defect research community. But not only them: the whole modern technology uses defects such as impurities and intrinsic structural imperfections for the development of the modern electronics which guarantees the creation of a wonderful digital new world (hopefully different from the *Brave New World* predicted by Aldous Huxley in 1932).

However, what appeared to be a utopia 50 years ago as well – artificial two-, one- and zero-dimensional solids – is now at the centre of practical technology. And these materials are also necessarily imperfect. They contain defects introduced during the synthesis or posterior modification by thermal or radiation treatment or maybe during exploitation. The variety of such materials and respective devices is quite impressive, and the Symposium "Defect-Induced Effects in Nanomaterials" held online from May 31st to June 3rd, 2021 in the framework of the E-MRS Spring meeting was the fifth edition of the event since the first one organized in 2012 in Warsaw. All five editions collected far more than 100 abstracts, demonstrating an undying interest in the issue. The program of the 2021 symposium comprised a total of 18 invited and 57 oral talks, as well as 71 poster presentations. The presenters came from 35 countries located on 6 continents: Africa, Asia, Europe, North and South America, and Oceania.

Twelve presentations have been selected for publication in a dedicated Special Section of *physica status solidi (b)*. The main defect-related hot topics covered by the articles are as follows.

Ab initio calculations:

E. Kotomin et al., V. Gusakov et al., and R. Maji et al. used *ab initio* calculations to describe the thermal stability and recombination kinetics of primary anion Frenkel defects – the F and F^+ electronic centres and oxygen interstitials – in fast-neutron-irradiated α-Al_2O_3 single crystals,[1] formation and diffusion of intrinsic defects in bulk and monolayer MoS_2,[2] and the interaction of grain boundaries (GB) with inherent defects and/or impurity elements in multi-crystalline Si,[3] respectively. The co-existence of two types of interstitials – neutral O atoms and negatively charged O ions – in α-Al_2O_3 has been demonstrated for the first time. Also for the first time, the formation energy of a split S and Mo Frenkel pair in bulk and monolayer MoS_2 has been obtained. The electronic properties of the considered Si-GB are not particularly affected by the strain and by the oxygen impurities unless a very high local distortion induces additional structural defects.

Antiphase boundaries:

Antiphase boundaries have also been investigated by G. Suchaneck et al. in $Sr_2FeMoO_{6-\delta}$,[4] and by M. Ananyev et al. in Sr-doped $LaScO_3$.[5] For the first time the weighted antiferromagnetic modulus, the bulk ferrimagnetic exchange stiffness constant, and the antiferromagnetic exchange stiffness constant across the antiphase boundary of $Sr_2FeMoO_{6-\delta}$ have been obtained by analyzing magnetoresistance data. The boundary width and boundary energy were calculated.[4] From the electron backscatter diffraction and transmission electron microscopy data, it has been concluded that $LaScO_3$ was homogeneous: there were no impurities and all the grains in the polycrystalline sample were structurally uniform and described in the framework of the same structural model of orthorhombic perovskite (space group Pnma).[5]

Radiation effects:

Z.T. Karipbayev et al. presented a study of the optical, structural, and mechanical properties of $Gd_3Ga_5O_{12}$ single crystals irradiated by $^{84}Kr^+$ ions.[6] The observed changes are ascribed to structural disturbances caused by depletion of the surface layer and an increase in the number of displaced atoms, accompanied by an increase in the crystal lattice parameter. C. Barone et al. combined measurements of broadband optical spectroscopy (10 meV to 6 eV), electrical resistivity and Hall effect to study the effects of gamma irradiation on electronic and optical properties of Ga-doped ZnO thin films.[7] High radiation hardness of the films has been found: the electrical resistivity, carrier concentration and electron mobility remain nearly unchanged, accompanied by minuscule changes of the optical properties.

Mechanical defects:

The growth of Al nanowires from mechanical defects on the black Al film surface is reported by M. Romanova et al.[8] Spiral-shaped Al nanowires grow from scratches and abrasions on the film surface already after heating up to 200 °C due to the stress-induced migration of aluminium atoms.

Spectroscopy of nanomaterials:

Luminescence and vacuum ultraviolet excitation spectroscopy of nanophosphors using synchrotron radiation has been performed by V. Pankratov et al.[9] It has been concluded that the size-dependent luminescence properties of nanophosphors are significant if the electron thermalization length becomes larger than the size of the nanoparticles. In this case, the multiplication of electronic excitations processes well-known in bulk materials is suppressed strongly in nanophosphors.

Positron annihilation spectroscopy:

The group led by H. Klym applied the positron annihilation lifetime spectroscopy to studies of the evolution of defect-related extended free volumes in chalcogenide glasses,[10] $MgAl_2O_4$ ceramics,[11] and $BaGa_2O_4$ ceramics doped with Eu^{3+} ions.[12]

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Agglomeration of free volumes in the initial stage of annealing with further fragmentation and shrinkage has been observed in the glasses. In the $MgAl_2O_4$ ceramics, the number and size of extended defects near grain boundaries have been found to decrease with the increasing sintering temperature, which correlates with the content of additional phases in materials. In the $BaGa_2O_4$ ceramics, the presence of Eu^{3+} ions results in the expansion of nanosized pores and an increase in their number with their future fragmentation.

The Symposium was a very exciting and fruitful event, a forum for reporting and discussing new findings, exchanging new ideas, and inspiring new concepts and designs. We hope that the present article collection will provide the reader with insights at least into some rapidly developing areas of the defect physics in nanomaterials.

We greatly acknowledge the financial and administrative support of the E-MRS Headquarters which allowed the successful organization of the symposium and the attraction of many young researchers from developing countries. Wiley-VCH kindly arranged the symposium publication.

The Guest Editors

[1] https://doi.org/10.1002/pssb.202100317
[2] https://doi.org/10.1002/pssb.202100479
[3] https://doi.org/10.1002/pssb.202100377
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