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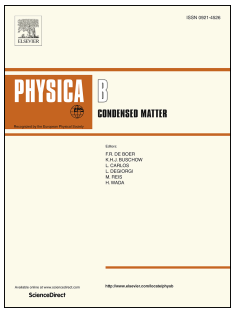

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Evidence of random distribution of carbon impurities in oxygen sites of zinc oxide

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Abstract. A density functional study of substitutional carbon impurities in ZnO-host matrix with 6.25 at. % was performed applying both the supercell method and the coherent potential approximation. The first of these methods assumes the spatially ordered arrangement of carbon impurities in oxygen sites, whereas the second one simulates the spatially disordered impurity substitution of oxygen sublattice. In conjunction with a theoretical part, the X-ray photoelectron spectra of pure and C-doped zinc oxide were measured. The mapping of the valence band of the carbon-loaded ZnO allows establishing the appearance of impurity C 2p electronic states on the valence band top. The experimental energy position of these impurity C 2p states is theoretically reproducing essentially better by the assumption about random distribution of carbon impurities in oxygen sublattice.

Keywords: density functional theory, coherent potential approximation, X-ray photoelectron spectra, carbon impurities, zinc oxide, random distribution of impurities.

1. Introduction

ZnO is one of the promising candidate for applications in ultraviolet (UV) optoelectronic devices because of its wide band gap (~3.37 eV) and large exciton binding energy (~60 meV) at room temperature. It can be used in the fields of blue and UV lasers, light-emitting diodes, solar cells [1, 2] and photo-electrochemical splitting of water for hydrogen production [3]. However, a wide intrinsic band gap of ZnO allows absorption of only UV light, which corresponds to 4 % of solar spectrum [4]. To extend the absorption spectrum of ZnO in visible region, the impurity doping was suggested. Instead of cationic doping in ZnO, anionic doping by nitrogen and carbon

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