Surface Modification of TiO_2 and ZnO Nanosurfaces and Applications

S. Y. Tong,[1,2]* Xu Hu,[1] R. Q Zhang, [1] M. K. Fung,[2] C. T. Yip,[2] A. M. C. Ng,[2] F. Fang,[2] A. B. Djurišić[2]
[1]Dept. of Physics and Materials Science, City University of Hong Kong, Tat Chee Avenue, Kowloon, Hong Kong
[2]Dept. of Physics, The University of Hong Kong, Pokfulam Road, Hong Kong
*E-mail: apdtong@cityu.edu.hk

***Abstract*-Nanomaterials are of great interest for a variety of practical applications. To achieve improved performance of nanomaterial-based devices it is essential to understand and modify their surface properties. Here we present an investigation of properties of nanosurfaces of ZnO and TiO_2, and discuss their applications in photovoltaics and antibacterial coatings.**

I. INTRODUCTION

Nanomaterials are of great interest for a variety of applications. In particular, metal oxide nanowires have been identified as very promising materials for applications in electronics, optoelectronics, and chemical sensing [1]. In addition to these applications, nanomaterials including metal oxides are present in a variety of consumer products, including sunscreens, toothpaste, textiles, etc. [2], and various nanomaterials are also actively investigated for antimicrobial applications [3]. To controllably and reproducibly prepare nanomaterials and nanomaterial-based devices with desired properties and performance, it is crucial to understand the fundamental properties of surfaces and interfaces due to inherently large surface-to-volume ratio of nanomaterials. While some progress has been made towards understanding the surfaces of bulk metal oxide samples [4-6], investigations of nanomaterial surfaces have been scarce.

We have studied the fundamental properties of TiO_2 and ZnO nanosurfaces using theory (ab initio total energy calculations, molecular dynamics simulations) and experiment (STM, LEED). While there is a wide range of applications of such studies, we will mainly report results of two applications, one is solar cells (PV) and the other is antibacterial coatings. In the case of solar cells, to achieve high efficiency it is necessary to minimize recombination losses by reducing the surface/interface defects which can serve as charge traps and recombination centers. We have studied both bare surfaces and passivated surfaces, and the obtained results are used to fabricate better functioning nanostructured photovoltaics. In the case of antibacterial coatings, we want to maximize the density of surface defects that can result in the generation of reactive oxygen species and thus increase the antibacterial activity of ZnO and TiO_2.

II. RESULTS AND DISCUSSION

ZnO and TiO_2 can be prepared using different methods, which result in a variety of morphologies, as well as a wide range of optical, electronic, and surface properties of the fabricated materials. In the case of ZnO, a great variation in morphologies and optical properties are often observed [7]. An example of ZnO nanorods grown on GaN film using different growth procedures is shown in Fig.1. It can be clearly observed that the growth method determines size, shape, and orientation of the nanorods. However, systematic studies which combine experiments with theoretical investigations of ZnO have been scarce.

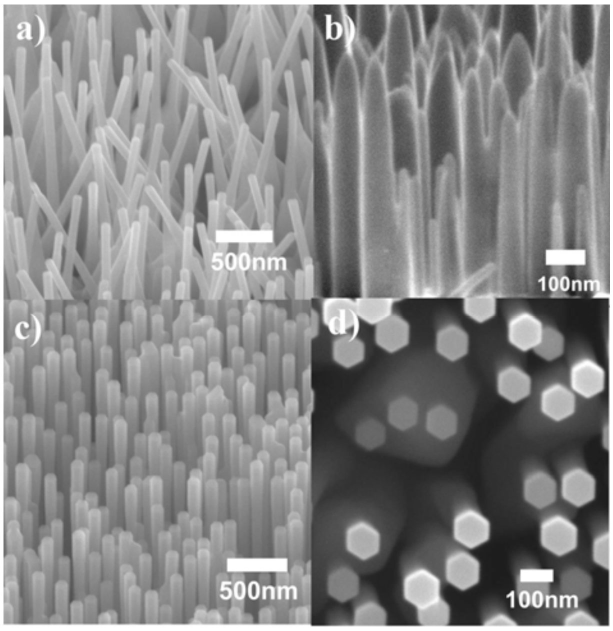

Fig. 1. a),b),c) Tilted view SEM images of ZnO nanorods grown on GaN using different growth conditions; d) Top view SEM image of the ZnO nanorod sample shown in tilted view c).

In the case of TiO_2, there is less variety of possible morphologies compared to ZnO. One of the commonly used morphologies are TiO_2 nanotube arrays due to their simple, low-cost fabrication by anodization [8,9]. An example of TiO_2 nanotube array is shown in Fig. 2. In this case as well, systematic studies to elucidate the relationship between fundamental surface properties of nanostructures and macrosopic material properties of nanostructure arrays have been scarce.

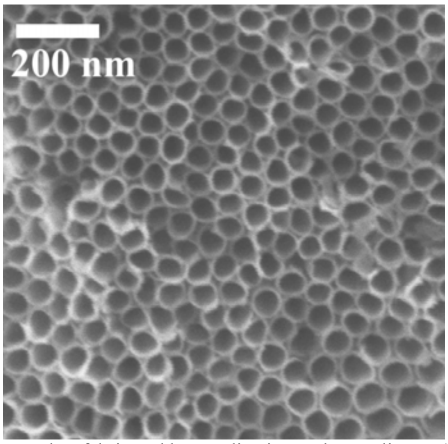

Fig. 2 TiO_2 nanotubes fabricated by anodization and annealing at 450ºC.

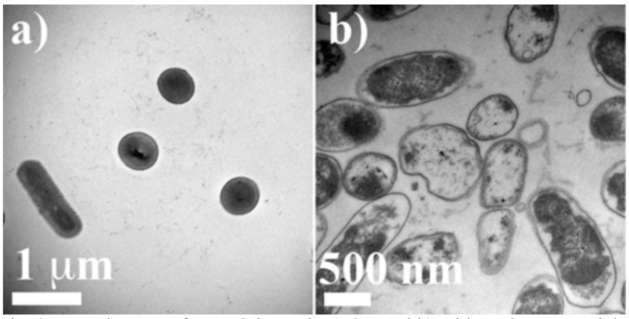

Fig. 3. TEM images of *E. Coli* bacteria a) Control b) with ZnO nanoparticles.

Therefore, we have studied fundamental properties of TiO_2 and ZnO nanosurfaces, and we discuss the implications of those properties on practical applications of these materials. We have selected two different applications, application in dye-sensitized solar cells [10] and as antibacterial coatings [11]. These applications have been selected since they have fundamentally opposite requirements for material properties. In photovoltaic applications, it is necessary to minimize recombination losses and improve dye adsorption, which requires minimization of traps and defects which can serve as recombination sites and thus negatively affect the power conversion efficiency. In the case of antibacterial application, reactive surfaces are needed, which would result in higher generation of reactive oxygen species in solution, and this can result in damage of cell walls and antibacterial activity, as illustrated in Fig. 3.

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