Institute for Plasma Research

Title:	Ion Beam Induced Modification of Wetting and Optoelectronic
	Properties of Functional Nanomaterials
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Abstract

Nanomaterials' novel characteristics and capabilities have ushered in a new era in a wide range of technical fields. Because of their exceptional electrical, optical, and thermal capabilities, these materials are intriguing for usage in a diverse array of applications. These nanomaterials have been very useful for solar cells, an important technology for renewable energy generation. Moreover, there are serious issues with stability of these materials due to strong interaction with moisture and not so efficient charge transport. In this report we are studying materials which are used in electron transport and hole transport layers (ETL/HTL) in perovskite based solar cells. Theses layers if made hydrophobic, can give good protection to the perovskite layer. On the other hand, these layers can be tuned to have better charge transport properties for better efficiency of the solar cell. There are several methods used to tune the ETL/HTL layers for such purpose. Surface wettability is adjusted for various uses by altering either the surface energy or the surface roughness, or both. Using an external agent is a reliable strategy for adjusting wettability. Due to stringent system requirements, many external agents/coatings have their own restrictions. The topography and chemistry of a surface can be altered through irradiation with energetic particles like electrons, ions, and neutrons. Exciting features of ion-solid interactions were uncovered by irradiating nanoparticles, which were not seen in bulk materials. Nanomaterials' high surface areas cause them to behave differently during sputtering, thermal spike-related effects, atomic diffusion, and annealing than bulk materials. In this report, the effects of ion beam irradiation on the structure, morphology, and chemistry of onedimensional (1D) metal oxide and two dimensional (2D) nanostructures, as well as their potential effects on the surface's wettability, were investigated. The effects of low energy ion beam irradiation on metal oxide functional nanomaterials (titanium dioxide, hematite), lead to better moisture repelling charge transport ability, can be used as ETL in Perovskite solar cells (PSCs). Irradiation causes modifications to the surface chemistry and electrical structure by introducing controlled defects, vacancies, and dopants. As a result, nanomaterials' wetting behavior can be drastically altered, leading to greater adhesion and compatibility with a wide range of surfaces. A state-of-the-art TRI3DYN simulation techniques has been used to study the ion-induced modification using Binary Collision Approximation based on Monte Carlo simulations. The water-solid interaction was investigated using the contact angle measurement instrument and the results were interpreted using density functional theory. In addition, the electrical conductivity of nanomaterials can be altered by irradiation with an ion beam due to the induction of structural flaws, grain boundary engineering, and local doping. My studies highlight that the low energy ion beam irradiation is an exceptionally helpful method for rapidly fabricating a moisture repelling and higher electrical conductive surface. These modified nanomaterials can be used as ETL/HTL layers and tuning work-function respectively in perovskite solar cell in future application.