【Grant-in-Aid for Scientific Research (S)】

Photovoltaic devices made of one-dimensional heterostructures

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Purpose and Background of the Research

●Outline of the Research

One-dimensional (1D) heterostructures consisting of single-walled carbon nanotubes (CNTs) coaxially stacked with different types of have been studied to elucidate the growth mechanism, extend atomic layer species, and evaluate optical and transport properties. In certain 1D heterostructures, different semiconductor layers inside and outside are electronically coupled through insulating layers, forming interlayer excitons. This leads to increased optical absorption, good electron-hole separation, and easy carrier transport within each semiconductor layer. Starting from CNTs with controlled structures, we will propose novel solar cells using thin films of 1D heterostructures through controlled synthesis and evaluation of optical and device characteristics.

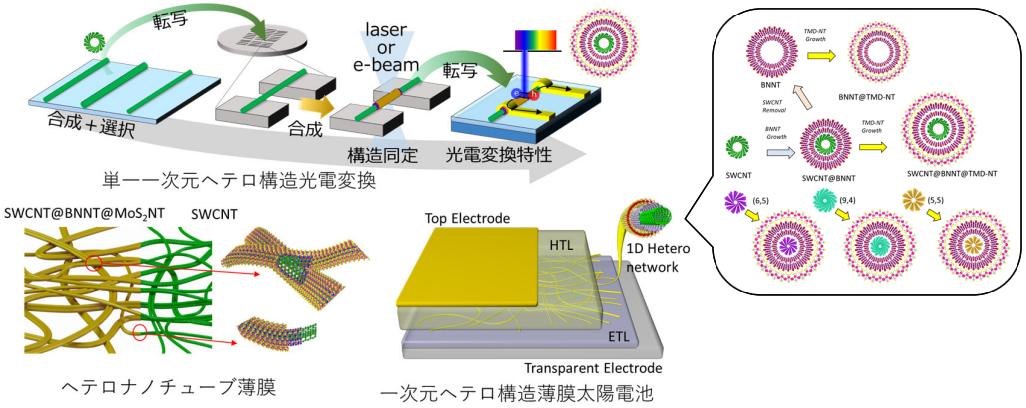

Figure 1. Schematic of a photovoltaic device based on a single heteronanotube and heteronanotube thin films. Starting from chirality-controlled SWCNTs, 1D heterostructures with various combination structures will be used.

●Background and purpose of research

Two-dimensional (2D) materials such as graphene, hexagonal boron nitride (h-BN), and transition metal dichalcogenides (TMDs) can form heterostructures through stacking due to van der Waals (vdW) forces. In fact, high-performance devices of graphene and TMDs have been realized by stacking between multilayer h-BNs. In 2D materials, heterostructures based on non-covalent vdW forces extend combinatorial freedom. Based on the stacking order of different atomic layers and the orientation angle, new physical phenomena emerge, pushing forward the research on 2D vdW heterostructures. In contrast, 1D nanotube materials exist, in which 2D materials are rounded into a tube-like structure, just as graphene corresponds to carbon nanotubes (CNTs). However, heterostructures combining different types of nanotubes have rarely been realized because while 2D materials can be easily obtained in small areas using mechanical exfoliation methods, no such method exists for nanotubes.

Recently, we proposed “1D heterostructures," extending the concept of vdW heterostructures to 1D, by using single-walled CNTs (SWCNTs) as templates to grow different atomic layers coaxially. An example is heteronanotubes with boron nitride nanotubes (BNNT) on the outer side and transition metal dichalcogenide nanotubes (TMD-NT) on the outermost (Figure 2). The realization of various combinations of atomic layers and functional design that exploits their physical properties may lead to innovative electronic, optical, and photovoltaic devices. In this project, we focus on interlayer excitons formed between the innermost SWCNT layer and the outermost TMD-NT layer to demonstrate 1D heterostructures in photovoltaic devices. We aim to propose an innovative thin-film solar cell system by starting with semiconducting or chirality-controlled SWCNT thin films.

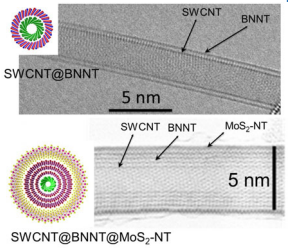

Figure 2. 1D vdW heterostructure with BNNTs formed around SWCNTs (top) and a three-layer heterostructure with additional MoS_2-NTs (bottom)

Expected Research Achievements

●How to conduct research

To realize 1D heterostructure photovoltaic devices composed of SWCNTs with constant chirality, BNNTs, and various TMDs, we will prepare SWCNT templates, synthesize heterostructures, and characterize their atomic structures, and electronic states. Also, we will evaluate the modulation of physical properties, interlayer excitons, and photo-voltaic properties due to the interaction of different nanotubes in 1Dl heterostructures. Based on these understandings, we will investigate the potential of using hetero-structure thin films of high-purity SWCNTs with optimal chirality distribution as active layers in solar cells. Specific research topics are 1. synthesis control and evaluation of 1D heterostructures, 2. evaluation of their physical properties, and 3. fabrication and evaluation of photovoltaic devices using 1D heterostructures.

●Expected outcomes and implications

Just like 2D vdW heterostructures, research on 1D counterparts is developing rapidly with high expectations. For 1D vdW heterostructures, we are interested in the optical properties that suggest a strong electronic coupling between SWCNTs and TMD-NTs in the outer layer via tunnel-layer BNNTs. For ‘2D materials' made of similar materials, the band structure is modulated by rolling into a nanotube structure, but in the case of typical MoS2-NTs, they are strongly coupled to the inner layer SWCNTs and inter-tube exciton) is also observed. In conventional 1D heterostructure assemblies, the heterogeneity of SWCNT bundles has limited observation of their optical properties and elucidation of their physical mechanism. In this study, we use our expertise in the synthesis control and handling of SWCNTs, based on isolated air-suspended SWCNTs and chirality-selected SWCNT ultrathin films, together with high-resolution electron microscopy and optical measurements, and to utilize first-principle calculations and various optical spectroscopy techniques to investigate the unique properties of 1D vdW heterostructures.

●Research team

Figure 3 shows the research team and the expected roles of each group. We have been performing various collaborative research. We will carry out our research by making the most of each research expertise.

Figure 3. Roles of each research group.

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