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Review

Oxide-free hybrid silicon nanowires: From fundamentals to applied nanotechnology

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ABSTRACT

The ability to control physical properties of silicon nanowires (Si NWs) by designing their surface bonds is important for their applicability in devices in the areas of nano-electronics, nano-photonics, including photovoltaics and sensing. In principle a wealth of different molecules can be attached to the bare Si NW surface atoms to create e.g. Si–O, Si–C, Si–N, etc. to mention just the most prominent ones. Si–O bond formation, i.e. oxidation usually takes place automatically as soon as Si NWs are exposed to ambient conditions and this is undesired is since a defective oxide layer (i.e. native silicon dioxide – SiO_2) can cause uncontrolled trap states in the band gap of silicon. Surface functionalization of Si NW surfaces with the aim to avoid oxidation can be carried out by permitting e.g. Si–C bond formation when alkyl chains are covalently attached to the Si NW surfaces by employing a versatile two-step chlorination/alkylation process that does not affect the original length and diameter of the NWs. Termination of Si NWs with alkyl molecules through covalent Si–C bonds can provide long term stability against oxidation of the Si NW surfaces. The alkyl chain length determines the molecular coverage of Si NW surfaces and thus the surface energy and next to simple Si–C bonds even bond types such as C=C and C≡C can be realized. When integrating differently functionalized Si NWs in functional devices such as field effect transistors (FETs) and solar cells, the physical properties of the resultant devices vary.

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Contents

1. Introduction

Much effort has been devoted to developing new nanomaterial-based technological devices with significant performance improvements at a reduced cost [1–4]. In this quest, a substantial number of nanomaterials have been developed, including but not limited to nanoparticles [5–14], nanorods [15–18], and nanowires [18–25]. Nanowires provide additional advantages compared to the other nanostructures in terms of their strong light absorbance, efficient charge separation and direct charge transport path. This makes them a promising candidate for many technological applications. In short, nanowires are important one-dimensional nanostructures that have demonstrated advantageous characteristics for applications in electronics [26–28], photovoltaics [29] and sensing [30–33].

Up till now, nanowires of many different inorganic materials have been synthesized and characterized, including silicon [34], gallium nitride [35] and lead selenide [18,36] among others. The use of silicon nanowires (Si NWs) in particular to further miniaturize devices while avoiding major process changes and their corresponding costs has been a topic of much research in the past decade. Thus, Si NWs are generally considered to be an essential class of nanodevice building blocks [37–39]. Si NWs have shown significant potential for field effect transistors (FETs). Potential applications of Si NWs in FETs includes aligning on insulating substrate surface, selective deposition of the source and drain contacts on the Si NW edges, and the configuration of either a bottom or top gate electrode [26,40]. Another significant potential application of Si NWs is solar power generation. The indirect optical band gap of 1.12 eV, low absorption co-efficient of 10^4/cm and high wafer cost of bulk Si reduces the suitability of this material for photovoltaic and optoelectronic devices. Differently engineered band gaps (1.4 eV) and a high absorption co-efficient (at least 10^5/cm) are required to significantly improve the solar cell efficiency. Si NWs are promising alternatives to bulk Si for use in solar cell applications due to their high light harvest; convenient band gap tuneability from 1.1 to 1.4 eV, which is achievable through decreases in the diameter [41]; and the possibility of fabricating the structures with a axial and lateral junction to decrease the charge bath separation [25,42–44].

Surface treatment is one of the main obstacles to Si NW application. A large body of chemistry has been developed for chemically linking moieties to oxidized Si NW surfaces, generally through –OH