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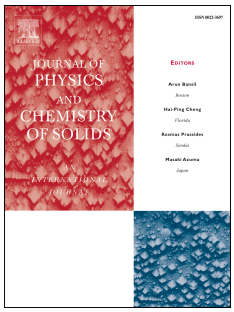

Influence of adsorbate and defect on structural and electronic properties of ultrathin silver nanotube

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PII: S0022-3697(17)30792-8

DOI: 10.1016/j.jpcs.2017.07.031

Reference: PCS 8149

To appear in: *Journal of Physics and Chemistry of Solids*

Received Date: 8 May 2017

Revised Date: 6 July 2017

Accepted Date: 30 July 2017

Please cite this article as: L.-C. Ma, X.-Z. Wang, L. Ma, J.-M. Zhang, Influence of adsorbate and defect on structural and electronic properties of ultrathin silver nanotube, *Journal of Physics and Chemistry of Solids* (2017), doi: 10.1016/j.jpcs.2017.07.031.

Influence of adsorbate and defect on structural and electronic properties of ultrathin silver nanotube

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Abstract: Using first-principles calculations based on density-functional theory, the effects of adsorbates (CO molecule, O and N atoms) and defects (an adhered atom and a monovacancy) on structural and electronic properties of the smallest (4, 4) AgNT have been systematically investigated. For CO adsorption on energetically preferred top site, the donation–backdonation process between the CO and Ag states leads to the formation of bonding/antibonding pairs, $5\sigma_b/5\sigma_a$ and $2\pi_b^*/2\pi_a^*$, and the quantum conductance of AgNT decreases by $1G_0$ after CO adsorption. Both O and N atoms strongly interact with AgNT after adsorption, leading to a $3G_0$ and $2G_0$ of drop in quantum conductance, respectively, for the AgNT. High adsorption energy of adhesion of one Ag atom and relatively low formation energy of a monovacancy suggest that these two types of defects are likely to occur in the fabrication of AgNT. The quantum conductance of the AgNT remains unchanged for adhesion of one Ag atom, but decreases by $1G_0$ when a monovacancy is present.

Keywords: Silver nanotube; Adsorption; Defect; Electronic property; First-principles calculation

1. Introduction

With the increasing miniaturization of electronic and mechanical devices, metal nanowires (NWs) and nanotubes (NTs) have attracted extensive interest due to their extraordinary physical and chemical properties as well as possible technological applications in nanoelectronic circuits and biological nanosensors [1–4]. These NWs and NTs have displayed conductance quantization in units of $2e^2/h$ and ultimate NWs are one atom thick [5, 6]. The rapid progress in experimental techniques makes it possible to fabricate these metal quasi one-dimensional (1D) structures and measure their novel properties. Besides synthesizing the single Au atom chain suspended between two Au electrodes [5, 6], the helical multishell (HMS) AuNW and PtNW thinner than 2nm have been observed in the ultrahigh vacuum-transmission electron microscopy (UHV-TEM) experiments

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