Control on the physico-chemical properties of the Si nanowires surface

R. A. Puglisi,[1,*] C. Bongiorno,[1] G. Borgh,[2] E. Fazio,[2] C. Garozzo,[1] G. Mannino,[1] F. Neri,[2] G. Pellegrino,[1] S. Scalese[1] and A. La Magna.[1]

[1]*CNR Istituto per la Microelettronica e Microsistemi, Strada Ottava 5, Zona Industriale, 95121 Catania, Italy.*

[2]*Dipartimento Scienze Matematiche ed Informatiche, Scienze Fisiche e Scienze della Terra, Università degli Studi di Messina, Viale F. Stagno d'Alcontres, 31, 98166 Messina, Italy.*

*corresponding author: rosaria.puglisi@imm.cnr.it

Si nanowires (Si-NWs) are widely studied for nano-electronics, for example in photovoltaics because they bring many advantages like waveguide action, improvement of the light harvesting, decoupling of the photon absorption from the carrier collection paths making the coupling with radiation more efficient, transformation of the band gap into a direct one via quantum size effects. VLS-CVD is the most widespread method of Si-NWs synthesis using gold (Au) as catalyst but Au particles remain on the tip of the Si-NWs at the end of the growth. This fact represents an issue because Au generates a deep acceptor state at Ec-0.54 eV in n-type Si and a donor level at Ev-0.35 eV in p-type Si that significantly reduce the device efficiency. Developing an effective method of Au removal is essential for the production of more efficient devices. Indeed, suggested methods are till now inefficient, oxidize the Si-NWs sidewalls or produce structural damage on the Si-NWs inner core. In this work, a physical-chemical characterization highlights that a 1-2 nm thick shell covering the Au tip acts as a barrier for the Au removal; a detailed studied of its chemical composition is presented. The layer formation is related to the heating/cooling and consequent phase separation processes taking place in the eutectic particles. A new approach fast and efficient for the Au removal is then proposed. The characterization after the chemical etching is also performed to check the eventual alterations in the Si-NWs morphological features and the removal efficiency.