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Coulomb Blockade Effect in Well-Arranged 2D Arrays of Palladium Nano-Islands for Hydrogen Detection at Room Temperature: A Modeling Study

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Abstract: The fast growth of hydrogen usage as a clean fuel in civil applications such as transportation, space technology, etc. highlights the importance of the reliable detection of its leakage and accumulation under explosion limit by sensors with a low power consumption at times when there is no accumulation of hydrogen in the environment. In this research, a new and efficient mechanism is presented for hydrogen detection—using the Coulomb blockade effect in a well-arranged 2D array of palladium nano-islands—which can operate at room temperature. We demonstrated that under certain conditions of size distribution and the regularity of palladium nano-islands, with selected sizes of 1.7, 3 and 6.1 nm, the blockade threshold will appear in current-voltage (IV) characteristics. In reality, it will be achieved by the inherent uncertainty in the size of the islands in nano-scale fabrication or by controlling the size of nanoparticles from 1.7 to 6.1 nm, considering a regular arrangement of nanoparticles that satisfies single-electron tunneling requirements. Based on the simulation results, the threshold voltage is shifted towards lower ones due to the expansion of Pd nanoparticles exposed to the environment with hydrogen concentrations lower than 2.6%. Also, exploring the features of the presented structure as a gas sensor, provides robustness against the Gaussian variation in nano-islands sizes and temperature variations. Remarkably, the existence of the threshold voltage in the IV curve and adjusting the bias voltage below this threshold leads to a drastic reduction in power consumption. There is also an improvement in the minimum detectable hydrogen concentration as well as the sensor response.

Keywords: Coulomb blockade threshold; hydrogen gas sensor; single-electron tunneling; palladium nanoparticles; room temperature

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