

Supporting Information

Flexible Chemiresistor Sensor with a Thin Film Assembly of Gold Nanoparticles: Responses to Volatile Organic Compounds under Device Strains

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1. Additional Experimental and Theoretical Details:

Additional Experimental Details: Following R2R fabrication of the flexible sensor devices, the etching process of the interdigitated copper microelectrode devices was carried out by controlled exposure through the etching solutions. Typically, it involved 210 seconds exposure to 110 g/L (0.46 M) Na₂S₂O₈ solution followed by 60 seconds exposure to a solution of 0.25 M basic KMnO₄ solutions mixed with 0.5 M NaOH. After removing photoresists the devices were thoroughly cleaned with deionized water.

For the thin film assembly of nanoparticles on the flexible device, the device was immersed into the solution of DT–Au_{2nm} (0.06 mM) nanoparticles and NDT (10 mM) at room temperature for a controlled period of time, during which the solvent evaporation was prevented in the film formation. The resulting film–coated device was rinsed many times to remove any un–assembled components, and dried using nitrogen gas. The thickness of the thin film was controlled by the assembly time.

Theoretical considerations: The electrical conductivity of the nanoparticle thin film assemblies in the absence of device strains has been found to follow the thermally–activated conduction pathway in which the activation energy increases with the interparticle distance and decreases with the particle size, details of which are described in our previous reports.^{S1–S3}

$$\sigma = \sigma_0 \exp(-\beta d) \exp\left[-\frac{0.5e^2}{4\pi\epsilon_{dielectric}\epsilon_0 RT} \left(\frac{1}{r_{np}} - \frac{1}{r_{np} + d}\right)\right] \quad (1)$$

where $e = 1.6 \times 10^{-19}$ C, $\epsilon_0 = 8.854 \times 10^{-12}$ F/m, $R = 1.38 \times 10^{-23}$ J/K, $T = 300$ K, β the electron coupling term, and r_{np} and d represent particle radius and interparticle spacing (nm), respectively.^{S3} We have recently shown^{S4} that under a simple device strain (ϵ_{strain}) for a nanoparticle thin film coated flexible PET substrate:

$$\epsilon_{Strain} = \frac{\Delta L}{L} = \frac{d_{bent} - d_{FL}}{2r_{np} + d_{FL}} = \frac{T_s}{2r_b} \quad (2)$$

where there is a length change from flat (d_{FL}) to bent (d_{bent}) is $\Delta L (=d_{bent}-d_{FL})$, $\Delta R/R_1$ can be derived as a function of strain ε_{strain} :

$$\begin{aligned} \frac{\Delta R}{R_{FL}} &= \frac{R_{bent} - R_{FL}}{R_{FL}} = \exp[-\beta(d_{FL} - d_{bent})] \exp\left[\frac{0.5e^2}{4\pi\varepsilon_{di}\varepsilon_0RT} \left(\frac{1}{r_{np} + d_{FL}} - \frac{1}{r_{np} + d_{bent}}\right)\right] - 1 \\ &= \exp[\beta(d_{FL} - d_{bent})] \exp\left[\frac{27.8nm}{\varepsilon_{di}} \times \left(\frac{1}{r_{np} + d_{FL}} - \frac{1}{r_{np} + d_{bent}}\right)\right] - 1 \\ &= \exp[\beta(2r_{np} + d_{FL})\varepsilon_{Strain}] \exp\left[\frac{27.8nm}{\varepsilon_{di}} \times \left(\frac{1}{r_{np} + d_{FL}} - \frac{1}{r_{np} + d_{FL} + \varepsilon_{Strain}(2r_{np} + d_{FL})}\right)\right] - 1 \end{aligned} \quad (3)$$

We have recently shown^{S4} that (1) $\Delta R/R_{FL}$ increases with ε_{strain} , (2) the magnitude of $\Delta R/R_{FL}$ is larger for tensile strain than that for compressive strain, (3) the magnitude of $\Delta R/R_{FL}$ depends on particle size and β value, and (4) the magnitude of $\Delta R/R_{FL}$ decreases with the increase of ε_{di} . By exploiting this sensitivity we are able to detect measurable changes in resistance that could result from even small modifications to the inter-particle distance from substrate straining. The gauge factor, g , is a scale of the sensitivity of a strain gauge and can be expressed as

$$g = \frac{\Delta R / R_{FL}}{\varepsilon_{strain}} = \frac{\Delta R / R_{FL}}{\Delta L / L} \quad (4)$$

where R and L are the resistance and sample length respectively. The gauge factor g depends on ε_{strain} for both convex (tensile strain) and concave (compressive strain) wrapping directions.

2. Additional Experimental Data:

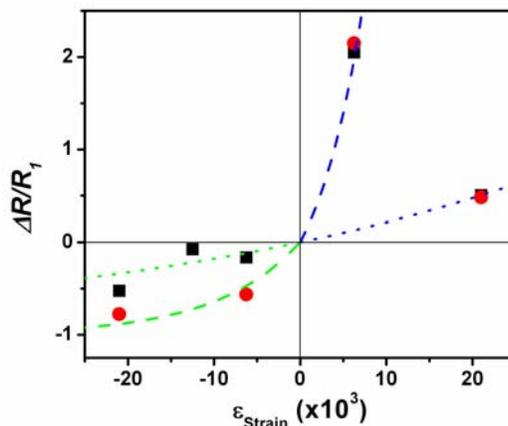


Figure S1. A comparison of the theoretical (based on eqn. 3) and the experimental data reported in the previous paper ($\Delta R/R_1 = \Delta R/R_{FL}$) [S4]. The dash/dot lines represent trends calculated from eqn. 3 ($r_{np} = 1.0$ nm, $d_{FL} = 1.6$ nm, $\varepsilon_{di} = 10$) under two types of strains. tensile strain: $\beta = 48$ nm⁻¹ (blue dash) and 5 nm⁻¹ (blue dot); and compressive strain: $\beta = 5$ nm⁻¹ (green dot), 28 nm⁻¹ (green dash).

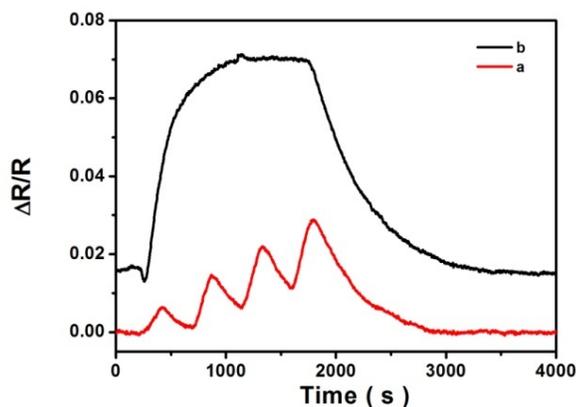


Figure S2. Response profiles ($\Delta R/R = \Delta R/R_{N_2}$) for a flexible chemiresistor device coated with an NDT-Au_{2nm} thin film in response to hexane at an exposure time of 2 mins (red, a: from left to right 826, 1652, 2478, 3304 ppm) and 10 mins (black, b: 2478 ppm).

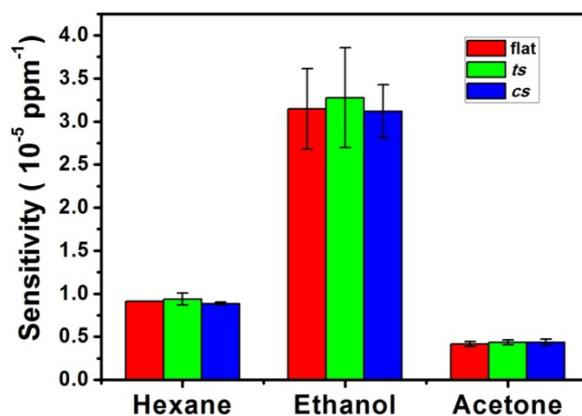


Figure S3. Average sensor response sensitivities for a chemiresistor device coated with an NDT-Au_{2nm} film in response to hexane, ethanol, and acetone under flat, tensile (*ts*) and compressive (*cs*) strains.

References:

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