Supplement information

Fiber-Tip Fabry-Pérot Interferometer with Graphene-Au-Pd Cantilever for Trace Hydrogen Sensing

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1. Sensor Fabrication

The fabrication process of the hydrogen sensor was divided into three steps: (1) Formation of the F-P cavity over the fiber tip with graphene; (2) Coating the fiber tip with Au and Pd for graphene-Au-Pd film; (3) Fabrication of cantilever on the graphene-Au-Pd film. The details are illustrated in Fig. S1.



Fig. S1 The fabrication process of the fiber-tip FPI with graphene-Au-Pd nanofilm-cantilever.

2. The determination of the Au thickness

The bending of the microcantilever is a response to the formation of surface stress caused by the adsorption of hydrogen molecules on the Pd film. the bending deflection of the nanofilm-cantilever due to hydrogen adsorption can be expressed as[1, 2]

$$Z = 3(\alpha_{Pd} - \alpha_f) \left(\frac{t_{Pd} + t_f}{t_f^2 k} \right) CL^2$$
(1)

where L is the length of the cantilever, t_{Pd} , t_f and α_{Pd} , α_f are the layer thicknesses and expansion coefficients, respectively. The subscript *f* refers to the nanocantilever foundation, which consisted of graphene film and Au film. *C* is the equilibrium concentration of the hydrogen atoms in the Pd nanofilm, the quantity *k* is determined by Young's moduli and thickness of the cantilever and Pd film [1].

$$k = 4 + 6\left(\frac{t_1}{t_2}\right) + 4\left(\frac{t_1}{t_2}\right)^2 + \left(\frac{E_1}{E_2}\right)\left(\frac{t_1}{t_2}\right)^3 + \left(\frac{E_2}{E_1}\right)\left(\frac{t_2}{t_1}\right)$$
(2)

We can deduce from the formula that as the Au film thickness increases, the deformation of the cantilever decreases, lowering the sensor's sensitivity. However, because the gold film also serves as a support film for the Pd film, it cannot be infinitely small. The thickness of the corresponding gold film is critical for making the Au film perform well in both functions at the same time.

In order to obtain the optimal Au film thickness, different thicknesses of Au films were used to prepare FPI hydrogen sensors. The thicknesses of Au films with coating times of 36 minutes, 72 minutes and 120 minutes are 141.17 nm, 252.40 nm and 396.45 nm, respectively, as shown in Fig S2. We compared SEM images of cantilever beams with different coating times (corresponding with different Au film thicknesses), as shown in Fig. S2. The samples with the 120-minutes coating (corresponding to a 400 nm Au film) demonstrated considerable mechanical properties. These experiments have demonstrated that a thickness of about 400 nm is preferred.



Fig. S2 The thicknesses of Au film and SEM imaging of graphene-Au-Pd cantilever with different Au coating time.

References:

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[2] C. Xiong, J. Zhou, C. Liao, M. Zhu, Y. Wang, S. Liu, C. Li, Y. Zhang, Y. Zhao, Z. Gan, L. Venturelli, S. Kasas, X. Zhang, G. Dietler and Y. Wang. Fiber-Tip Polymer Microcantilever for Fast and Highly Sensitive Hydrogen Measurement. *ACS applied materials & interfaces*, 2020, **12(29)**, 33163-33172.