Refractive Index Sensing with Plasmons in 2D Metals

Lei Kang, Yuhao Wu, Sawyer D. Campbell, and Douglas H. Werner

> Department of Electrical Engineering The Pennsylvania State University University Park, PA, 16802 USA dhw@psu.edu

Department of Materials Science and Engineering, Department of Physics, Department of Chemistry, Center for Nanoscale Science, 2D Crystal Consortium, Center for Atomically Thin Multifunctional Coatings, Center for 2D and Layered Materials The Pennsylvania State University

University Park, PA, 16802 USA

Joshua A. Robinson

Abstract— In this paper, we show that nano-engineered ultrathin two-dimensional (2D) metal films supporting infrared plasmonic resonances can enable highly responsive refractive index (RI) sensing. Our results reveal the strong dependence of the RI sensitivity on the 2D-metals' thickness. In particular, for a 1nm-thick analyte layer, a RI sensitivity up to 110 nm/RIU (90 nm/RIU) is observed in atomically thin 2D-In (2D-Ga) nanoribbons exhibiting highly localized plasmonic resonances at mid-infrared wavelengths.

Keywords— 2D metals; plasmons; field-enhancement; midinfrared; refractive index sensing

I. INTRODUCTION

Plasmonic sensors offering label-free refractive index (RI) detection have been of considerable interest. In the perturbation regime, the corresponding RI sensitivity (S_{RI}) is proportional to the resonant field distributions and the volume of the analyte region. In other words, S_{RI} is simultaneously determined by the local field concentration and the overlap of the field with the analyte. Accordingly, an analyte layer of a characteristic thickness of hundreds of nanometers is generally required for conventional plasmonic sensors operating at visible and near-IR wavelengths [1].

Recent studies show that ultra-thin and 2D metals can support strong plasmons, leading to tight field confinement and large field enhancement at the metal-dielectric interface. The corresponding plasmonic resonances are expected to be extremely sensitive to the dielectric environment, which makes 2D-metal nanostructures an excellent platform for highly responsive RI sensing. The recent development of confinement heteroepitaxy (CHet), based on intercalation of metallic elements at the graphene/SiC interface, provides a new approach to the synthesis of large-area atomically thin polar metal heterostructures (PMets) with precisely controlled thickness. Protected by graphene overlayers, the crystalline 2D polar metals are excellent candidates for plasmonic devices. In particular, the permittivity dispersions of 2D-Ga and 2D-In suggest plasmon frequencies in the near-IR region, implying that the two material systems can support strong plasmonic responses in the near- to mid-infrared spectral range.

In this paper, we numerically study the RI sensing capability of nanoribbon structures of ultra-thin gold, 2D-Ga, and 2D-In which support infrared plasmonic resonances. In particular, based on the plasmonic resonance at wavelengths around 1600 nm, 3-nm-Au nanoribbons exhibit an $S_{RI} > 650$ nm/RIU for a 100-nm-thick analyte layer. The strong dependence of the S_{RI} on the 2D-metals' thickness is observed. Furthermore, a 2D-In (2D-Ga) nanoribbon plasmonic sensor can enable sensing of a 1-nmthick analyte with an S_{RI} up to 110 nm/RIU (90 nm/RIU). Our study reveals the remarkable sensing capability of 2D-metal systems, suggesting the potential of 2D-metal-based plasmonic devices for enhanced IR detection.

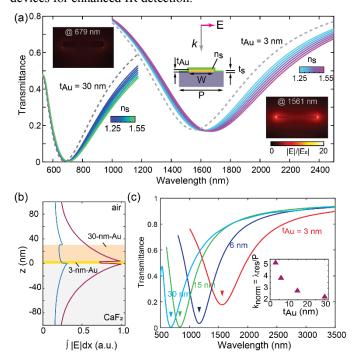


Fig. 1. Refractive index sensing enabled by infrared plasmons in ultrathin metals. (a) Transmittance spectra of the Au nanoribbon ($\bar{W} = 200 \text{ nm}, P = 1.5W$) sensing system when $t_{Au} = 3$ nm, $t_s = 10$ nm. The transmittance spectra of a (conventional) system of the same geometries but with $t_{Au} = 30$ nm are also presented. Insets: on-resonance electric field distributions. (b) Normalized field integration in a unit cell in the z direction. (c) Transmittance spectra of Au nanoribbons for different thicknesses ($t_{Au} = 3$ nm, 6 nm, 15 nm, and 30 nm). Inset: k_{norm} of the corresponding resonances as a function of t_{Au} .

II. SIMULATIONS

A periodic ultra-thin Au nanoribbon array ($t_{Au} = 3$ nm) located on top of a CaF₂ substrate ($\varepsilon_{\text{CaF2}} = 2.03$) is considered (Fig. 1(a)). A conformal cover layer (of thickness t_s) serves as the analyte with a refractive index n_s . Simulated transmittance spectra shown in Fig. 1(a) indicate a pronounced redshift of the resonance when n_s of the 10-nm-thick analyte layer increases from 1.25 to 1.55. In contrast, only a trivial variation is observed in the spectra of the conventional sensing system ($t_{Au} = 30$ nm). This distinct sensing performance can be attributed to the plasmon excitation in the ultra-thin Au nanostructures. This is made evident from the electric field distributions at the resonance wavelength of the two systems (insets in Fig. 1(a)). In addition, the electric field integration within a unit cell (Fig. 1(c)) unambiguously shows the Au-thickness-dependent field enhancement effect. To better illustrate this thickness-effect, Fig. 1(d) displays the transmittance spectra of nanoribbons for different Au thicknesses ($t_{Au} = 3, 6, 15, \text{ and } 30 \text{ nm}$) with the inset summarizing the normalized wavenumber (k_{norm}) of the corresponding resonances as a function of t_{Au} .

The spectral shift of plasmonic resonances due to a change in both n_s and t_s of the analyte layer can be expressed as $\Delta \lambda = \partial \mathcal{N}(\partial n_s) \cdot \Delta n_s + \partial \mathcal{N}(\partial t_s) \cdot \Delta t_s$ [2]. Accordingly, we further study the sensitivity of the 3-nm-Au sensor where the corresponding results (Fig. 2) offer a complete picture of the sensing performance. A RI sensitivity $\partial \mathcal{N} \partial n = 655$ nm/RIU is observed at $t_s = 100$ nm, while for $t_s = 1$ nm, a thickness sensitivity of $\partial \mathcal{N} \partial t = 11$ nm/nm, which is ~ 20 times larger than that seen in photonic crystal slab sensors [3], is observed. Furthermore, the insets in Fig. 2(b) and (d) summarize the dependences of $\Delta \lambda$ and the resonance linewidth on n_s for the four systems of different Au thicknesses when $t_s = 2$ nm, which again reveals the strong thickness effect in such 2D-metal plasmonic sensors.

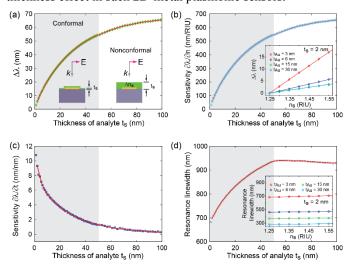


Fig. 2. Sensitivity study of the sensor based on 3-nm-Au nanoribbons. The dependence of (a) $\Delta\lambda$ when $\Delta n_s = 1.50 - 1.40$, (b) $\partial\lambda\partial n$, (c) $\partial\lambda\partial t$ ($n_s = 1.40$), and (d) resonance linewidth on the thickness of the analyte (t_s). Inset in (b) and (d): $\Delta\lambda$ and resonance linewidth as a function of n_s for systems with different t_{Au} when $t_s = 2$ nm.

By simply treating 2D-Ga and 2D-In as homogeneous and isotropic thin films with a thickness of 0.52 nm and 0.49 nm, respectively, we numerically study the 2D-Ga and 2D-In nanoribbon systems for RI sensing. Fig. 3(a) and (b) illustrate the corresponding transmittance spectra when $t_s = 10$ nm and n_s varies in a range from 1.25 to 1.55. The observed resonance shift

can be attributed to the plasmonic resonance supported by the system, which can be seen from the on-resonance electric field distributions (insets in Fig. 3(a) and (b)). In addition, the t_s -dependences depicted in Fig. 3(c) and (d) provide a comprehensive sensitivity comparison between the sensing systems based on 3-nm-Au, 2D-Ga, and 2D-In nanoribbons.

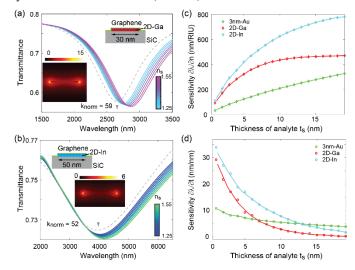


Fig. 3. Mid-IR RI sensing based on plasmons in 2D polar metals. Transmittance spectra corresponding to (a) 2D-Ga and (b) 2D-In nanoribbons. Insets: electric field distributions at a resonance wavelength of 2654 nm (2D-Ga) and (d) 3927 nm (2D-In). The dependence of (c) $\partial \mathcal{N} \partial n$ and (d) $\partial \mathcal{N} \partial t$ on t_s . For comparison, the results for a 3-nm-Au system are also presented.

III. CONCLUSION

In summary, we have numerically validate that 2D-metal nanostructures supporting plasmonic resonances can enable plasmon-enhanced refractive index sensing. The corresponding high sensitivity can be attributed to the plasmon-induced strong field confinement and enhancement effect at the surface of 2D metals due to the thickness-effect.

ACKNOWLEDGMENT

This work was funded by the DARPA EXTREME program under award #HR00111720032. This work was also supported by the National Science Foundation, under NSF DMR-2002651 and the Penn State MRSEC, Center for Nanoscale Science, under the award NSF DMR-2011839.

REFERENCES

- [1] T. Weiss, et al., "From dark to bright: First-order perturbation theory with analytical mode normalization for plasmonic nanoantenna arrays applied to refractive index sensing," Phys. Rev. Lett., vol. 116, no. 23, 237401 (1-4), Jun. 2016.
- [2] Y. Sun and X. Fan, "Analysis of ring resonators for chemical vapor sensor development," Opt. Express, vol. 16, no. 14, pp. 10254-10268, Jun. 2008.
- [3] Y. Liu, et al., "Optofluidic vapor sensing with free-space coupled 2D photonic crystal slabs," Sci. Rep., vol. 9, pp. 4209 (1-8), Mar. 2019.
- [4] N. Briggs, et al., "Atomically thin half-van der Waals metals enabled by confinement heteroepitaxy," Nat. Mater., vol. 19, pp. 637-643, Jun. 2020.