Measured and Simulated Optical Transmission Through Nanoholes in a Bilayer of Gold and Vanadium Dioxide

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We investigate optical transmission through hybrid nanohole arrays that combine the plasmonic behavior of a nanopatterned gold (Au) film with the switching functionality of a vanadium dioxide (VO_2) film, which exhibits a reversible semiconductor-to-metal transition at convenient temperatures (T_c ~ 67 °C) and its optical properties undergo large hysteretic changes. The aim of this work was to fabricate some previously simulated[1] Au+VO_2 nanohole arrays and measure their transmission spectra, in order to determine if the large metallic-to-semiconducting switching ratio of the primary transmission peaks, simulated in each phase for the optimized nanohole array (M2S-ratio ~ 200; see bottom panel of Fig. 1(a)), would survive under real-world fabrication and measurement conditions. We find that experimental non-idealities, such as incomplete perforation of the VO_2 layer (compare Fig. 1(a) and 1(c)) or conical instead of cylindrical depth profile of the holes (not shown here), significantly affect the relative magnitude of the transmission peaks across the VO_2 phase transition. The six arrays, each consisting of several thousand nanoscale holes of various diameters and periodicities (Fig. 1 lists the nominal values), were milled on a Raith Velion FIB-SEM system. Prior to the milling process, we deposited a 245-nm VO_2 film on glass by pulsed laser deposition and crystallized it by rapid thermal annealing, followed by sputter-deposition of a 200-nm Au film. We measured many VIS-NIR transmission spectra, some of which are shown in Fig. 1(b), as a function of temperature through the six arrays, as well as through unperforated VO_2 and Au+VO_2 areas, and then constructed the thermal hysteresis for each recorded wavelength. We also performed finite-element method computations with varying hole depths and shapes, which greatly affect the relative transmission through the hole arrays. For instance, transmission in the semiconducting state increases when the VO_2 layer is perforated only halfway through. Measurements and simulations both showed that peak transmission through Au+VO_2 holes was almost always higher for metallic VO_2—opposite to the behavior of the *unperforated* VO_2 film and Au+VO_2 bilayer. We will discuss this counterintuitive 'reverse switching' effect, the influence of geometrical parameters on the spectra, non-monotonic hysteresis loops (e.g., note that the 67 °C spectra in Fig. 1(b) are lower than the corresponding 30 °C spectra), and a prominent spectral feature that appears in the measurements (broad shoulder peak past 800 nm) but not in the simulations.

[1] E. U. Donev, F. X. Hart, B. I. Nkurunziza, K. Bertschinger, J. Zhang, and J. Y. Suh, "Parametric study of optical transmission through plasmonic hole arrays modulated by the phase transition of vanadium dioxide," *OSA Continuum* **3**, 2106–2133 (2020); 10.1364/OSAC.390879.

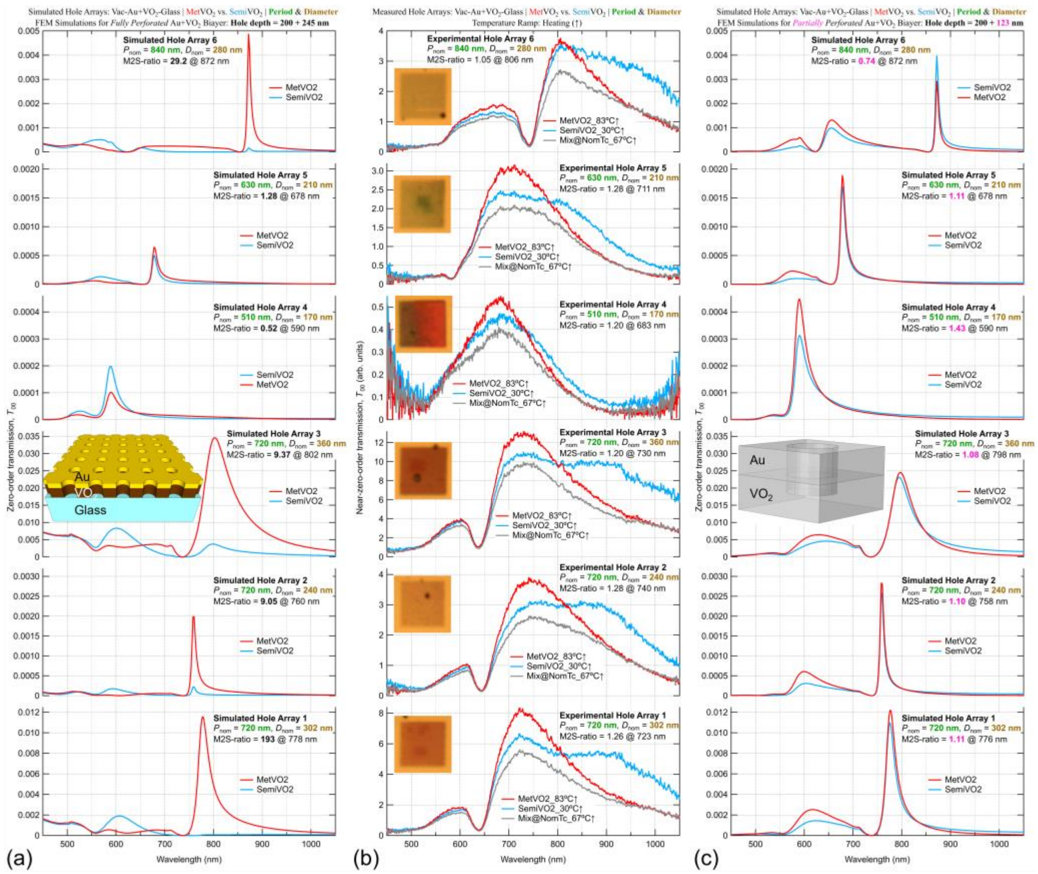

Figure 1: Measured and simulated optical transmission spectra through six periodic arrays of nanoholes perforating a bilayer of gold (Au, 200 nm) and vanadium dioxide (VO_2, 245 nm) thin films. **(a)** Simulated zero-order transmission spectra, in the metallic and semiconducting states, using the nominal geometric parameters of the six nanohole arrays in (b) and assuming a fully perforated VO_2 layer (i.e., no residual VO_2 in the holes); (inset) schematic of a fully perforated Au+VO_2 bilayer on a glass substrate. **(b)** Near-zero-order transmission spectra, taken at three temperatures (30°C/semiconducting, 67°C/mixed-phase, 83°C/metallic) across the VO_2 phase transition: three arrays of the same nominal periodicity (720 nm) but different nominal hole diameters (from bottom: 302, 240, 360 nm) and three arrays of different nominal periodicities and hole diameters (from top: 840/280, 630/210, 510/170 nm); (insets) optical micrographs of the six 50×50 μm^2 arrays. **(c)** Similar to (a) except assuming a half-perforated VO_2 layer (i.e., a 122.5-nm residual layer of intact VO_2 material at the bottom of each hole); (inset) partial geometry of the unit cell from the finite-element method (FEM) model (COMSOL Multiphysics). **Bottom line:** Possible incomplete milling of the VO_2 layer appears to substantially affect the transmission in the semiconducting state, which may explain why the experimental metallic-to-semiconducting (M2S) peak transmission ratios (legends in (b)) are much closer to their simulated counterparts in the case of half-milled holes (legends in (c)) versus thru-holes (legends in (a)).