High-quality factor Ta₂O₅-on-insulator resonators with ultimate thermal stability

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Experiments in photonics, laser optics and quantum technology require low loss, thermal and mechanical stability. While photonic integrated circuits on monolithic chips achieve interferometric stability, important nanophotonic material systems suffer from propagation loss, thermal drift and noise that prevent, for example, precise frequency stabilization of resonators. Here we show that tantalum pentoxide (Ta_2O_5) on insulator micro-ring resonators combine quality factors beyond 1.8 Mio. with vanishing temperature-dependent wavelength shift in the relevant 70 K to 90 K temperature range. Our Ta₂O₅-on-SiO₂ devices will thus enable athermal operation at liquid nitrogen temperatures, paving the way for ultra-stable low-cost resonators, as desired for wavelength division multiplexing, on chip frequency stabilization and low noise optical frequency comb generation.

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Performing experiments in ultra-low noise environments has become a crucial requirement in many branches of optics. State-5 of-the-art optical clocks, precision spectroscopy, nonlinear optics, 6 and quantum technology implementations are extremely sensi-7 tive to both mechanical noise as well as thermal noise processes. This is exemplified by the enormous challenges involved in laser frequency stabilization with ultra-high quality factor (Q) 10 Fabry-Perot cavities fabricated from ultra-low expansion glasses 11 or even single crystal materials [1–3]. Photonic integrated cir-12 cuits (PICs) allow for overcoming mechanical stability issues 13 by fabricating resonators out of dielectric thin film systems on 14 monolithic chips. While low cost and small device footprints due 15 to strong mode confinement in high refractive index dielectrics 16 constitute some advantages over bulk optic implementations, 17 most PIC resonators suffer from noise introduced by variations 18 in humidity, pressure, and, most importantly, temperature [4, 5]. 19 20 The corresponding thermo-refractive noise of a PIC resonator is directly dependent on the thermo-optic and thermal expansion 21 22 coefficients of the respective nanophotonic material system [6]. To realize stable micro-resonators with high quality factors a PIC platform further needs to achieve ultra-low optical loss.

Here we show that Tantalum Pentoxide-on-insulator (Ta_2O_5) PICs can satisfy these challenging demands when cooled to liquid nitrogen temperatures. Ta2O5 is emerging as a CMOS compatible nanophotonic material platform with optical properties that uniquely benefit a broad range of applications in metrology, nonlinear optics and quantum technologies [7–11]. Importantly, Ta_2O_5 offers high refractive index contrast to SiO₂, resulting in stable nanophotonic devices with compact footprints due to strong mode confinement [12-14]. Ta₂O₅ further features a wide transparency window from the ultraviolet to the infrared (0.28 µm-8 µm) [15], extremely low levels of intrinsic material fluorescence under optical excitation [16], negligible two photon absorption [17], and a relatively large third order optical nonlinearity. These features have allowed quantum emitter integration into Ta2O5 waveguides and the demonstration of nonlinear optical effects such as super continuum generation and spontaneous four wave mixing [18–21]. However, all applications to date have focused on room temperature operation, where thermorefractive noise in Ta₂O₅-on-SiO₂ is comparable to other established nanophotonic platforms. Here, we investigate Ta₂O₅ on insulator micro-ring resonators over a large temperature range, extending the device operation down to 3 K. At liquid nitrogen temperatures we find minimal Temperature Dependent Wavelength Shift (TDWS) for wavelengths in the telecommunication C-band, thus giving rise to a new class of temperature stable high quality-factor devices with relaxed cooling requirements.

We assess the thermal stability of Ta_2O_5 PICs by extracting the TDWS of high-quality factor micro-ring resonances, which are cooled from room temperature to 3 K in a closed cycle cryostat. We employ spectroscopic ellipsometry (SE) of the Ta_2O_5 -on-SiO₂ sample over a similar temperature range to determine the thermal expansion coefficient and then extract the thermo-optic coefficient from the TDWS measurements. This technique allows for separating the contributions of (Ta_2O_5) waveguide and (SiO_2) substrate on the thermal behavior of the device.

To best assess the intrinsic properties of Ta_2O_5 devices, we design micro-ring resonators for multi-mode operation, featuring wider waveguides in which fundamental propagation modes



Fig. 1. (a) Refractive index of a Ta_2O_5 thin film, determined via multilayer modeling of spectroscopic ellipsometry. (inset) Simulated optical mode profile in a Ta₂O₅ ridge waveguide (b) FEM simulations of effective refractive indices for propagating modes in Ta₂O₅ waveguides of different width.

are less affected by scattering at waveguide sidewalls, leading 63 to higher quality factors. We first record variable angle spectro-64 scopic ellipsometer (VASE) data over a large wavelength range 65 101 from 350 nm – 1800 nm at room temperature (Woolam M-2000) 66 102 67 and fit a multilayer model to the ellipsometric spectra via regres-103 68 sion analysis [22]. This procedure allows for extracting optical 104 parameters such as refractive index $n(\lambda)$, extinction coefficient 69 105 $\kappa(\lambda)$ and film thickness for each layer, which constitute essential 70 106 input for nanophotonic device design. The resulting $n(\lambda)$ of 71 107 the Ta₂O₅ film with a nominal thickness of 330 nm is shown in 72 108 Figure 1 a. From electromagnetic field simulations using the 73 109 finite element method (FEM, Comsol Multiphysics), we find 74 110 that Ta₂O₅ waveguides of 330 nm \times 1.2 µm cross section on SiO₂ 75 111 substrates predominantly support the fundamental transverse 76 electric (TE00) mode at 1550 nm wavelength, as shown in the in-77 set of Figure 1 a, which we use as single-mode feed waveguides. 78 Multimode operation up to TE40, on the other hand, is possible 79 112 in waveguides of 4 µm width, as shown in Figure 1 b, which we 80 113 chose for the micro-ring resonators. To minimize bending loss, 81 we chose to work with a micro-ring diameter of 150 µm. 82 114

We fabricate the micro-ring resonator devices, as shown in 83 115 84 Figure 2 a, from 330 nm ion beam sputter deposited Ta_2O_5 thin 116 85 films on a 3.3 µm buried oxide layer on a silicon handle wafer 117 (thicknesses are nominal values). Grating couplers, waveguides 86 118 and micro-ring resonators are patterned via electron beam lithog-87 119 raphy using a negative tone photoresist (ma-N 2403, micro resist 88 120 technology) and reactive ion etching in CF₄-CHF₃-Ar chemistry. 121 89 Each sample is annealed in oxygen enriched N₂ atmosphere at 90 122 600 °C for 6 h, which was found to notably reduce propagation 91 123 loss of ion-beam sputtered Ta_2O_5 thin films [23–25], as can be 92 124 inferred from determining the Q-factors of micro-ring resonators 93 125 as a function of annealing temperature . 94

We characterize the resonator devices in transmission mea-127 95 surements with a sweep-laser in the telecom C-band (Toptica 128 96 CTL-1500), as shown in Figure 2 b. For measurements in the 300 129 97 K to 3 K temperature range the chip is mounted inside a closed 130 98 cycle cryostat (ICEOxford Dry ICE 1K) on a cryogenic 3-axes 131 99 translation stage (Attocube ANPxyz101). The setup allows for 132 100



Fig. 2. (a) Scanning electron micrograph of a Ta₂O₅-oninsulator ring resonator. (b) Setup for quality factor measurements and detection of the TDWS (c) Resonance spectrum of a ring resonator and corresponding resonator modes as extracted from the FSR. (d) Single resonance of a multimode waveguide with a loaded quality factor of approx. 1.8 Mio. The quality factor is obtained from fitting a Lorentzian line shape to the data.

positioning the grating couplers of a device under test under an optical fiber array, which also collects transmitted light for intensity measurements with a photodiode (NewFocus 2053-FC-M). The recorded spectra (see Figure 2 c) allow for identifying the modes guided inside the resonator by comparing experimentally observed free spectral ranges (FSR) with simulation results. For the TE00 mode we find loaded quality factors up to Q = 1.84Mio. from fitting a Lorentzian function to the data acquired with slightly over-coupled devices at room temperature, as shown in Figure 2 d.

The TDWS, given as [26]

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$$\Delta \lambda \sim \frac{n_{\rm eff} \alpha}{n_{\rm eff,g}} \lambda \Delta T \tag{1}$$

describes fluctuation of the resonance wavelength λ of the microring in terms of device temperature and the coefficient of thermal expansion (CTE) α that follows a $\frac{1}{L} \times \left(\frac{\delta L}{\delta T}\right)$ dependence on optical path length L inside the resonator. Here it is noteworthy that the optical mode extends from the Ta2O5 waveguide into the SiO₂ substrate (see Figure 1 a inset) and both material components contribute to the TDWS. We experimentally determine the TDWS $\Delta\lambda$ by following the center wavelength of a single high Qfactor resonance when cooling the chip from room temperature to 3 K.

The data in Figure 3 a shows the resonance wavelength as determined from a Lorentzian fit to the transmitted power data for a large number of temperature values, measured at the backside of the sample. The TDWS is here expressed relative to the resonance wavelength at 3 K. Notably the gradient of the TDWS vanishes not only for temperatures < 15 K, where several quantum technology devices are being operated, but also in the 70 K - 90 K temperature range, which can conveniently be reached with economic liquid nitrogen (LN) cooling. In these temperature regions Ta₂O₅-on-SiO₂ devices achieve ultimate thermal stability.



Fig. 3. (a) TDWS vs temperature. The measured resonance wavelength at 3 K serves as a reference for the TDWS at other temperatures. The inset shows a zoom in to temperature range around 80 K where the TDWS-gradient changes sign. (b) Refractive index of a Ta₂O₅ thin film for different temperatures determined from SE measurements (Accurion ellipsometer) from 1.5 K to room temperature. The data measured with the Woollam ellipsometer (same as Figure 1 a) is plotted to show the close agreement of the results from two different Ellipsometers accessing different wavelength ranges.



Fig. 4. ((a) Refractive index of the SiO₂ substrate for different temperatures, measured from 1.5 K to room temperature with the Accurion SE. The data for SiO₂ and Ta₂O₅ are determined from the same ellipsometer measurement, thus enabling effective refractive index simulations. (b) Effective refractive index simulated via FEM for 1.2 μ m wide, 330 nm thick Ta₂O₅-on-SiO₂ waveguides.

To investigate the origin of this behavior, we combine the 161 133 aforementioned room temperature SE measurements over large 162 134 spectral bandwidth (see Figure 1 a) with temperature depen- 163 135 dent SE measurements performed with a customized Accurion 164 136 EP4 spectroscopic imaging ellipsometer, covering the 450 nm 165 13 1000 nm spectral range. The ellipsometer is combined with 166 138 a closed cycle cryostat with an adiabatic demagnetization re- 167 139 frigerating (ADR) stage (Kiutra S-Type Optical) with a special 168 140 designed, home-built cold-finger and vacuum can. The vacuum 141 can and radiation shields are equipped with windows for direct 170 142 optical access. The angle of incidence used in the temperature 171 143 dependent SE measurements was fixed to 50° and is adjusted 144 to the window configuration of the cryostat in order to ensure 172 145 orthogonal light beams through the windows to avoid their im- 173 146 pact on SE measurements while maintaining suitable reflectance 174 147 contrast between s- and p- polarized light. 175 148

The refractive indices $n(\lambda)$ for the thin films are again de- 177 149 termined from fits to the measured SE spectra using the same 178 150 multilayer model as for spectrally extended room temperature 151 179 Woollam SE measurements. To model the SiO₂ film a Sellmeier 152 180 term, as an improvement of the classical Cauchy function, was 153 181 used and for the Ta₂O₅ film a combination of a Tauc-Lorentz 154 182 term, a UV-pole and an Eps-fix term was employed [27]. The 155 Tauc-Lorentz term is a refinement of the Lorentz oscillator model 156 describing the lowest direct interband transition. The UV-pole 185 157 represents a pole in the real part of the dielectric function describ- 186 158 ing higher lying interband transitions far from the experimental 187 159 accessible energy range still influencing the linear light-matter 160

interaction in the measured wavelength range. The Eps-fix term establishes the light dispersion in the high-energy limit with ϵ_{∞} . The wavelength resolved refractive indices $n(\lambda)$ for Ta₂O₅ and SiO₂ thin films for the temperature range from 1.5 K to room temperature are shown in Figure 3 b and Figure 4 a, respectively. The extracted film thicknesses from fits to the model with typical root mean squared error (RMSE) values of 8 from regression analysis are rather constant in the investigated temperature range and yield 3.49 µm for SiO₂ and 318 nm for Ta₂O₅, respectively, which is within the fabrication tolerances of the nominal thickness values .

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Extrapolation of the temperature dependent data into the telecom C-band, where no low-temperature compatible ellipsometry capabilities were available to us, is accompanied by increasing uncertainties. We however recognize that the dispersion function is flat in this wavelength regime and no wavelengthdependent variations of the relative differences in the temperature dependencies of the refractive index $n_{\lambda}(T)$ for fixed wavelengths λ occur in the experimentally utilized wavelength range from 700 nm to 1000 nm, as seen in Figure 3 b. We further find that FEM simulations, similar to those shown in Figure 1, but based on low-temperature ellipsometry data, yield effective refractive indices for our nanophotonic devices that show vanishing gradients in a temperature range that coincides with the findings in TDWS measurements (see Figure 4 b). For these FEM simulations we neglect the CTE, which accounts for strain of all materials in the layer stack. Such treatment is adequate because the 525 µm thick silicon substrate contributes by far the

largest material portion as compared to the $3.3 \,\mu m \, SiO_2$ and 189 $330 \text{ nm } \text{Ta}_2\text{O}_5$ thin films [28]. We note that the CTE of the sili-250 190 con substrate is on the order of $1 \times 10^{-6} \text{ K}^{-1}$ [29, 30], leading 191 252 to a variation of a few nanometers over the 300 K temperature 192 253 range, which has negligible influence on the effective refractive 193 254 194 index of a nanophotonic device. In addition, SiO₂ and Ta₂O₅ are 255 195 rather soft amorphous films and hence much less prone to strain 256 caused by lattice mismatch. 196 257

On the other hand, the CTE has a noticeable effect on the 197 258 coupling conditions and the free spectral range of the resonator 259 198 even for small changes of the microring radius. Consequently, 200 199 the thermal expansion coefficient α contributes considerably to ²⁶¹ 200 262 the TDWS depicted in Figure 3 a. The corresponding functional 20 263 behavior of the TDWS (see also Figure 4 b) resembles that of 202 the slope of the expansion of silicon with a minimum at 85 K 203 [29, 30]. From Equation 1 we conclude that the product of the 204 266 CTE and the effective refractive index results in a shift of the 205 267 global minimum in agreement with our measured TDWS. With 206 268 effective refractive index and CTE reaching minimal values at 207 269 73 K and 85 K, respectively, we find optimal thermal device 270 208 stability at 81.5 K. Realizations of thermally stable devices, such 271 209 as the resonators considered here, will further benefit from slow 272 210 variations of CTE, effective refractive index and TDWS around 273 211 274 their respective minimal values, thus providing stable operation 212 275 over an extended temperature range. 213 276

In summary, we show that Ta₂O₅-on-insulator photonic in-214 277 tegrated circuits allow for combining low-loss waveguiding 215 278 with ultimate thermal stability. Optimal thermal conditions 216 279 are found at 81.5K by investigating the TDWS of a cryogeni-217 280 cally cooled micro-ring resonator with loaded quality factors 281 218 in excess of 1.8 Mio. Spectroscopic ellipsometry under cryo- 282 219 genic conditions provides evidence for the contributions of the 283 220 temperature-dependent effective refractive index and CTE to the 284 221 TWDS. Our results establish the Ta2O5-on-insulator nanopho- 285 222 286 tonic platform as an ideal choice for a wide range of applications 223 287 requiring ultimate thermal stability, which is straightforwardly 224 288 achievable at cost-efficient liquid nitrogen temperatures. 225 289

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 Data Availability Statement. Data underlying the results presented in this paper are not publicly available at this time but may be obtained from the authors upon reasonable request.
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