

Chemical passivation of GaAs (100) using alkanethiols

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III-V semiconductors are among the most promising materials for low-power and high-speed electronic devices owing to their high electron mobility and high breakdown fields. For instance, their use as channel materials would enable an increase in performance without changing the transistor density. Despite these advantages, III-V materials lack a defect-free and stable native oxide that could be used as a dielectric in metal-oxide-semiconductor field-effect transistors (MOSFET).¹ Moreover, the most widely studied III-V semiconductor, GaAs, contains interfacial oxides that detrimentally affect its electronic performance. The native oxide of GaAs is mainly composed of As³⁺, As⁵⁺, Ga¹⁺, and Ga³⁺ states, which need to be removed in order to render the substrate suitable for electronic applications.

One approach involves the chemical etching of these oxides and the deposition of a passivation layer that hinders further oxidation. Etching of GaAs oxide states can be carried out using NH₄OH, H₂SO₄-H₂O₂ mixtures, HF, or HCl in aqueous solutions.^{2,3,4,5} On the other hand, chemical passivation with layers containing S have shown particular promise and have been deposited using the precursors Na₂S, (NH₄)₂S, or alkanethiols.^{5,6,7} If the thiol molecules can be closely packed, the alkyl chain on the thiols can act as a diffusion barrier to prevent oxygen from reaching the III-V surface.

In this study, etching of GaAs oxide states was accomplished by a sequential treatment with HF, H₂O₂, and HCl. Alkanethiols with chain lengths from 3-20 carbon atoms (Fig. 1) were deposited from the liquid phase on GaAs (100), and their effectiveness in preventing oxidation in ambient conditions was characterized using ellipsometry, X-ray photoelectron spectroscopy (XPS), and Fourier-transform infrared spectroscopy (FTIR). Ellipsometry and C 1s XPS peak showed that thiols with longer carbon chains exhibited larger thickness (Fig. 2) and higher surface coverage, respectively. After short exposure times (3 minutes) samples treated with short thiol molecules exhibited rapid oxidation, while long thiols reduced below detection limits the oxide states of both As and Ga (Fig. 3). Oxidation of the substrate was also prevented by a thiol with 20 carbon atoms after relatively long exposure times (30 minutes). FTIR peaks at 2918±1 and 2850±1 cm⁻¹, corresponding to asymmetric and symmetric stretches of CH₂ groups, demonstrated the formation of a well ordered monolayer for chains with 18 and 20 carbon atoms (Fig. 4a). In addition, XPS and temperature programmed desorption (TPD) confirmed the successful desorption of the carbon chains of thiols after annealing in vacuum to 750 K (Fig. 4b). Atomic layer deposition (ALD) of Al₂O₃ using a TMA and water process showed that film nucleation and growth was reduced by a factor of about two on the thiol-passivated surface compared to the liquid-cleaned surface (Fig. 4c). Although the initial film growth was slowed, a thiol passivation layer could broaden the use of III-V semiconductors in device manufacturing.

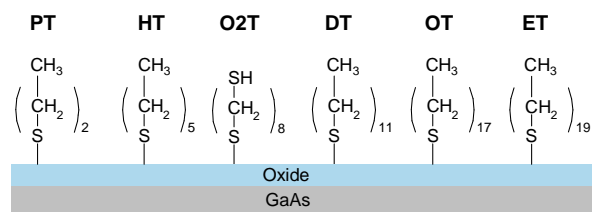


Figure 1. Scheme of 1-propanethiol (PT), 1-hexanethiol (HT), 1,8-octanedithiol (O2T), 1-dodecanethiol (DT), 1-octadecanethiol (OT), and 1-eicosanethiol (ET) deposition on GaAs.

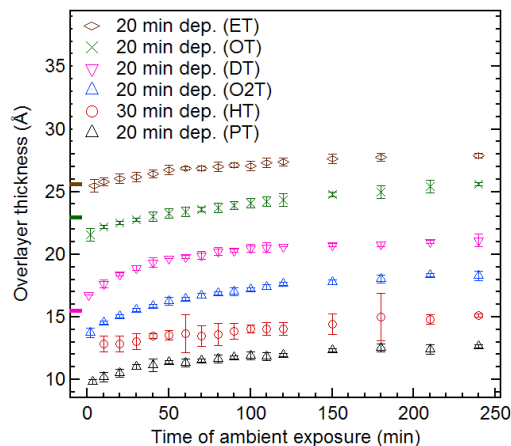


Figure 2. Ellipsometric thickness of the overlayer (alkanethiol and GaAs oxides) after thiol deposition.

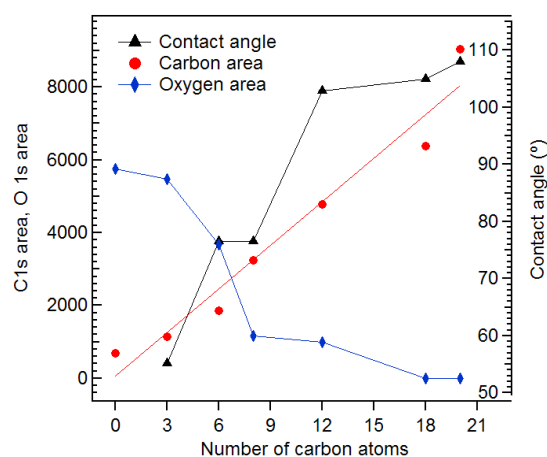


Figure 3. Water contact angle, C 1s XPS peak, and O 1s XPS peak areas after passivation. Solid lines are guides to the eye.

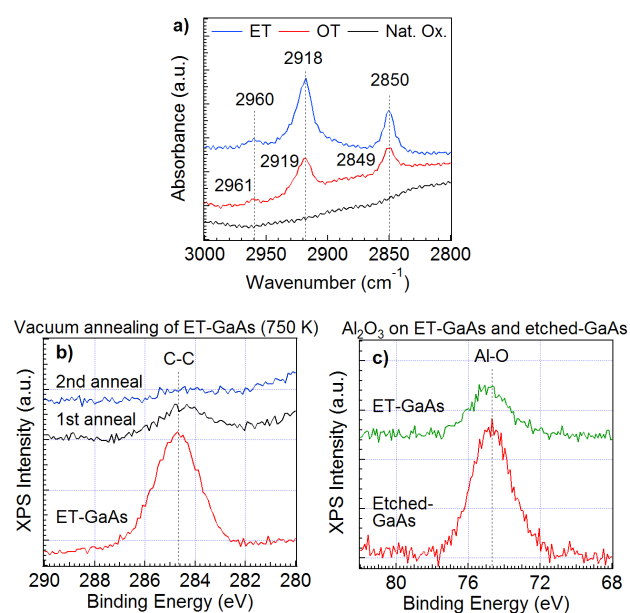


Figure 4. a) Transmission FTIR of passivated GaAs, b) XPS before and after TPD, and c) ALD of Al₂O₃ on passivated and non-passivated GaAs.

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