Supporting information for

Nitride surface passivation of GaAs nanowires: impact on surface state density.

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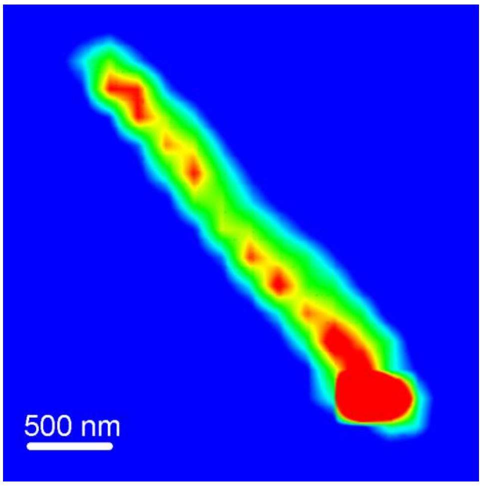

Figure S1. μ-PL intensity distribution (at wavelength λ = 870 nm, 300 K) over the surface of nitrided *n*-GaAs NW lying horizontally on a Si substrate covered by a Si_3N_4 film. As it seen, the intensity distribution is uniform along NW.

CALCULATION DETAILS

The passivation-induced increase of the PL intensity (I_{PL}) observed for lightly doped NWs provides evidence of the broadening of a non-depleted core inside the NWs, where the radiative recombination of photoexcited excess carriers is possible. For unpassivated NW under a constant pumping level $I_{PL1} \propto r_1^2$, where r_1 is the radius of the non-depleted core. The radius of the non-depleted core in the nitrided NW r_2 can be simply estimated, provided that r_1, $r_2 << r$ where r is the radius of the NW, from the following expression

$$I_{PL2}/I_{PL1}=r_2^2/r_1^2 = 6. \qquad (1)$$

Thus one can conclude that the surface nitridation produces the 2.5- fold increase of the radius of the non-depleted core. Figure S2 presents a schematic picture of energy diagrams with the conduction channels for unpassivated (Fig. S2 a) and nitrided (Fig. S2 b) NWs under light excitation.

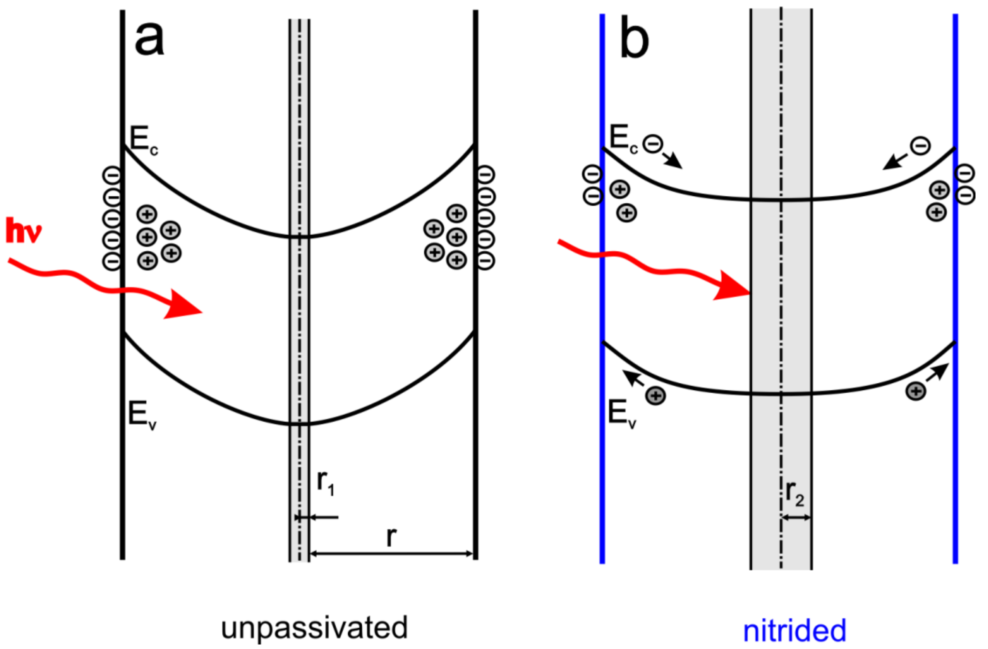

Figure S2. Energy band diagrams with conduction channels for: (a) unpassivated and (b) nitrided NWs under light excitation.

We find the dependence of the radius r_1 on the surface recombination velocity S_r. Under photoexcitation by a monochromatic light with the wavelength λ incident on a NW perpendicularly to its axis, the photogeneration rate G is linearly proportional to the photoexcitation intensity I_0:

$$G = \alpha I_0. \qquad (2)$$

where α is optical absorption coefficient for the NW material at given wavelength λ. Thus, for the case $\alpha^{-1} >> 2r$, the photogeneration rate can be assumed to be constant over the whole NW volume. Then the total number of the excess carriers generated in the NW volume V per unit time is

$$q_G = GV = \pi\alpha I_0 \ell r^2 \quad . \qquad (3)$$

Next, the photogenerated excess holes occur to be in electric field of the depletion area at the NW surface, which, as has been already mentioned above, covers the whole NW volume. In a NW with n-type background doping, the holes drift in electric field of the depletion area towards NW surface, where they recombine with the electrons occupying the respective surface states. As far as the diffusion length of the minority carriers (holes) in lightly doped NW occurs to be greater than the NW radius, one can assume that nearly all excess holes (except those, which recombine radiatively with excess electrons inside the NW and contribute to the PL) can reach the NW surface.

The total number of holes recombining at NW surface per unit time:

$$q_s = S_r \Delta p_s S, \qquad (4)$$

where $S = 2\pi r\ell$ is total area of the NW side surface, Δp_s is concentration of the excess holes at NW surface. In steady state regime, $q_s = q_G$. Neglecting the recombination inside NW, one obtains from (3) and (4):

$$\Delta p_s = \frac{q_G}{S_r S} = \frac{\alpha I_0 r}{2S_r} \quad . \qquad (5)$$

Then, the total nonequilibrium charge of the NW near-surface layer with thickness $w_0 << r$ can be written as[1]

$$\Delta Q_\mathrm{s} = \frac{e\Delta p_\mathrm{s} S w_0}{2} = \frac{\pi e \alpha I_0 \ell r^2 w_0}{2S_r} \ , \qquad (6)$$

where e is the electron charge.

The excess surface charge ΔQ_s reduces the surface barrier height due to surface photovoltage effect, which in turn decreases a thickness of depletion area. The excess charge ΔQ_s compensates the nonequilibrum charge ΔQ_i in the depletion area of width $r - r_1$. The latter charge can be written in the following form

$$\Delta Q_\mathrm{i} = \pi e N_\mathrm{d} \ell \left[r^2 - \left(r^2 - r_1^2 \right) \right] \ . \qquad (7)$$

Equating (6) and (7) one can obtain the radius of the non-depleted core at the center of NW under photoexcitation:

$$r_1^2 = \frac{\pi \alpha I_0 r^2 w_0}{2N_\mathrm{d} S_\mathrm{r}} \ . \qquad (8)$$

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[1]The nornalizing length w_0 is introduced to coordinate the dimensionality of the surface charge density Δp_s with the dimensionality of the surface recombination rate S_r, which is usually [cm×s^{-1}]. Physically, w_0 can be treated as a decay length of the envelope wave functions of the holes, trapped on surface states.

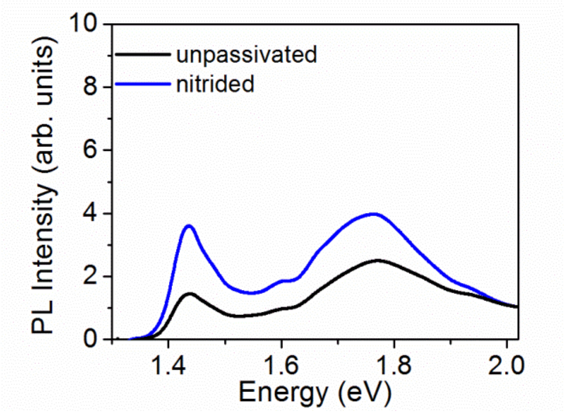

Figure S3. μ-PL spectra (300 K) taken from the middle parts of the nitrided, and unpassivated p^+ NWs. Note, that the peak at 1.77 eV presents in the spectra. Also half width of 1.42 peak for p^+ NW is larger than that for lightly doped n-NW by a factor of 1.5.

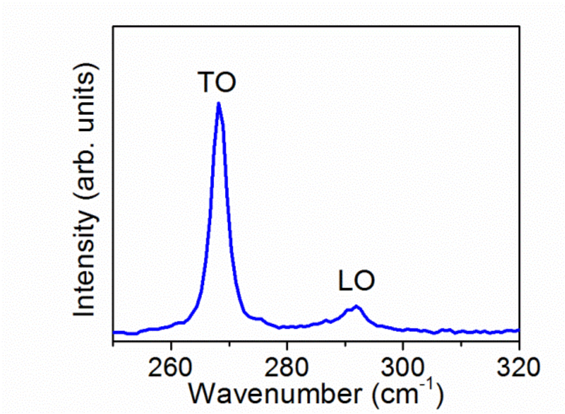

Figure S4. Raman spectra surface of nitrided *n*-GaAs NW lying horizontally on a Si substrate covered by a Si_3N_4 film.