Quantitative description of photo-excited scanning tunnelling spectroscopy

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Photo-excited scanning tunneling spectroscopy on *p*-doped nonpolar GaAs(110) surfaces exhibits an increased tunnel current at negative sample voltages under illumination. In order to analyze the experimental data quantitatively, the potential and charge-carrier distributions of the photo-excited tip-vacuum-semiconductor system are calculated by solving the Poisson as well as the hole and electron continuity equations by a finite-difference algorithm. The occupation of (resonant) surface states is taken into account. Tunnel currents are calculated using an extension of the model of Feenstra and Stroscio to include light-excited carrier concentrations. For negative sample voltages, the tunnel current is composed of a valence band contribution and photo-excited electrons that are tunneling from the conduction band into the tip.

The efficiency of solar cell and optoelectronic devices is closely connected to the nanoscale distribution of charge carriers. For example, defects can give rise to non-radiative carrier recombination centers, reducing the charge-carrier concentration locally [1,2]. Such effects are detrimental to both the electron-light and light-electron conversion efficiencies in optoelectronic and solar cell devices, respectively. In order to understand the physical processes involved at the atomic scale, the materials used in the device structures need to be investigated simultaneously under illumination and with atomic resolution.

Photo-excited scanning tunneling spectroscopy (STS) is ideally suited to probe the illumination-induced local surface photo-voltage, band bending, carrier concentration, and the electrostatic potential distribution with atomic resolution [1-7]. For a quantitative analysis, particularly of the local charge-carrier concentration and redistribution, a fundamental physical understanding and theoretical modelling of the photo-excited tunneling spectra is needed. Therefore, we present a generally applicable and detailed three-dimensional quantitative description of photo-excited STS [8].

Experiments were performed on freshly cleaved, clean, and atomically flat GaAs(110) surfaces ([Zn]= 2×10^{18} cm^{-3}). We used a 1mW laser diode exhibiting a wavelength of 785 nm. Estimations of the laser spot size at the sample surface and loses due to reflection at the surface and transmission through window flanges lead to an average irradiance of $(1.45 \pm 0.44) \times 10^{5}$ Wm^{-2}.

During the acquisition of current-voltage spectra, the laser was electrically modulated by the STS control electronics. In contrast to standard current-voltage spectra, we consecutively measured the current with and without illumination at each voltage step. Each of these steps took 1280 µs, during which first the laser was turned on for 180 µs only to minimize thermal drift. Second, the current without illumination was then acquired 800 µs after turning off the laser. Importantly, the current-voltage spectra with and without illumination were hence probed at the same tip-sample separation, which was fixed by the set voltage and current without illumination.

The resulting $I(V)$ spectra with (red squares) and without (black triangles) illumination are illustrated in Fig. 1. First, the onset voltage of the conduction band current I_C (at positive sample voltages) remains unchanged under illumination. This is due to upward band bending, screened with and without illumination by the accumulation of majority carriers at the surface. Therefore, the upward band bending is not altered significantly under illumination and the tunnel current remains essentially unchanged. Second, the onset voltage of the valence band current I_V (negative sample voltages) is shifted towards smaller negative voltages by $\delta V_{onset} \approx +0.2$ V under illumination. This indicates the presence of light-excited minority carriers at the semiconductor surface, whose concentration is orders of magnitude higher than that of thermally generated minority carriers. These minority carriers, on the one hand, can directly tunnel into the tip. On the other hand, they may enhance the screening, reducing the downward band bending at negative voltages under illumination and hence increasing the valence band tunnel current. The relative magnitude of these two effects is unclear and needs to be investigated quantitatively.

For this purpose we have developed a quantitative description of light-excited STS [8]. It is based on the three-dimensional solution of the Poisson- and the continuity equations for the tip-vacuum-semiconductor system employing a finite-difference algorithm [9]. The electron and hole current densities within the semiconductor are described by a drift-diffusion model. Continuity conditions for the electrostatic potential at the

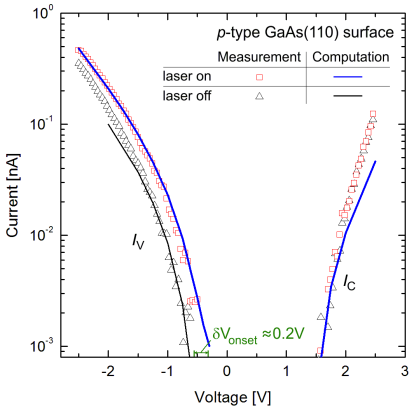

FIG. 1: I(V) spectra obtained on a p-doped GaAs(110) surface with (red squares) and without (black triangles) illumination for identical tip-sample separations. The set point is −2.0 V and 150 pA (without illumination). Without laser excitation the current at positive (negative) voltages arises from electrons tunneling into the conduction band labeled I_C (out of the valence band, I_V) [12]. The laser excitation increases the tunnel current at negative sample voltages only. The tunnel current is then composed of a valence band current and a photo-induced tunnel current. Computational results are shown as black (without illumination) and blue (with illumination) solid lines. Note, all the calculated spectra coincide at positive voltages.

semiconductor-vacuum interface are used to account for surface states - although it is generally known that the GaAs(110) surface is free of intrinsic surface states within the fundamental band gap, it was shown that resonant surface states can influence the tip-induced band bending and hence the tunnel current at this surface [10]. For the partial differential equations we assume Neumann boundary conditions. Photo-excited carriers are modelled by band-to-band generation and recombination terms. The metal tip is assumed to be hyperbolically shaped. For the derivation of the tunnel current, the electrostatic potential along the central axis (through the tip-apex) is used in a one-dimensional tunnel current model developed by Feenstra and Stroscio [11] that is extended by quasi Fermi-levels to account for tunnelling of photo-excited carriers. A complete description of the theoretical model is beyond the scope of this article, but can be found in [8].

For our calculations we use a tip radius of 20 nm and literature values for all further material parameters. The tip-sample separation was the only fit parameter for the calculation of the tunnel spectrum under dark conditions. We obtained the best fit of the calculated current (black solid line in Fig.1) to the experimental data for a tip-sample separation of 0.925 nm. For the fit of the tunnel current under illumination (blue solid line in Fig.1), the irradiance was the only fit parameter. The best fit was then obtained for an irradiance of $(1^{+0.7}_{-0.3}) \times 10^{-5}$ Wm^{-2} in good agreement with the experimentally observed value. The underlying model assumes a tip-induced band bending (cf. cross-sectional plots in Fig.2 (a)), which is limited by photo-excited electrons in the bulk and a partial occupation of the C_3 surface state (empty dangling bond state localized above the Ga surface atoms) due to light-excited electrons. The tunnel current at negative voltages is then composed of a valence band contribution and a photo-induced tunnel current caused by excited electrons in the conduction band that tunnel into the tip. Calculations also show that the direct tunneling of photo-excited minority carriers from the conduction band to the tip is dominating the tunnel current at negative voltages. An increased current solely due to enhanced screening without tunneling of photo-excited carriers would require much larger laser irradiances than that experimentally used.

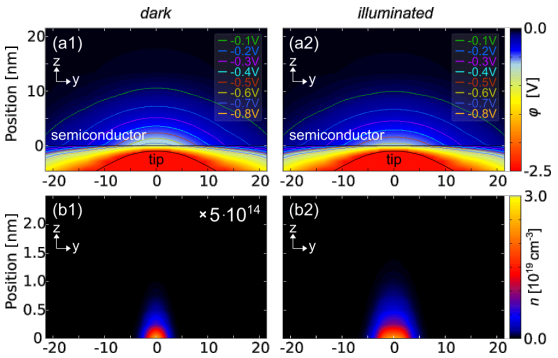

FIG. 2: Cross-sectional plots of (a) the electrostatic potential ϕ of the tip-vacuum-semiconductor system, (b) the electron concentration n (in the semiconductor only) for a sample voltage of −1.5 V without illumination (left column), and with illumination, photo-induced tunnel current, and surface-state limited band bending (right column). The equipotential lines in (a) range from −0.1 V to −0.8 V in steps of 0.1 V.

[1] R. J. Hamers and K. Markert, Phys. Rev. Lett. **64**, 1051 (1990).

[2] Y. Kuk, R. S. Becker, P. J. Silverman, and G. P. Kochanski, Phys. Rev. Lett. **65**, 456 (1990).

[3] T. W. Matthes, C. Sommerhalter, A. Rettenberger, M. Böhmisch, J. Boneberg, M. C. Lux-Steiner, and P. Leiderer, Applied Surf. Sci. **123/124**, 187 (1998)

[4] S. Aloni, I. Nevo, and G. Haase, Phys. Rev. B **60**, R2165 (1999).

[5] S. Yoshida, Y. Kanitani, R. Oshima, Y. Okada, O. Takeuchi, and H. Shigekawa, Phys. Rev. Lett. **98**, 026802 (2007).

[6] S. Yoshida, Y. Kanitani, R. Oshima, Y. Okada, O. Takeuchi, and H. Shigekawa, Jpn. J. Appl. Phys. **47**, 6117 (2008).

[7] S. Landrock, Y. Jiang, K. H. Wu, E. G. Wang, K. Urban, and Ph. Ebert, Appl. Phys. Lett. **95**, 072107 (2009).

[8] M. Schnedler, V. Portz, P. H. Weidlich, R. E. Dunin-Borkowski, and Ph. Ebert, Phys. Rev. B **91**, 235305 (2015).

[9] S. Selberherr, Analysis and Simulation of Semiconductor Devices (Springer, Vienna/New York, 1984)

[10] N. Ishida, K. Sueoka, and R. M. Feenstra, Phys. Rev. **B** 80, 075320 (2009).

[11] R. M. Feenstra and J. A. Stroscio, J. Vac. Sci. Technol. B **5**, 923 (1987).

[12] N. D. Jäger, E. R. Weber, K. Urban, and Ph. Ebert, Phys. Rev. B **67**, 165327 (2003).