

A new approach to modelling Kelvin probe force microscopy of hetero-structures in the dark and under illumination

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Abstract A numerical method is proposed to model Kelvin probe force microscopy of hetero-structures in the dark and under illumination. It is applied to FTO/TiO_2 and $FTO/TiO_2/MAPbI_3$ structures. The presence of surface states on the top of the TiO_2 layers are revealed by combining theoretical computation and experimental results. Basic features of Kelvin probe force microscopy under illumination, namely surface photovoltage, are simulated as well. The method paves the way toward further investigations of more complicated optoelectronic devices.

Keywords KPFM · Drift-diffusion · Hetero-structures · SPV · Halide perovskite

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As a combination of the Kelvin probe technique and the non-contact Atomic Force Microscope (AFM), the Kelvin Probe Force Microscope (KPFM) was first developed in 1991 (Rosenwaks et al. 2007), to indirectly infer interface electronic properties. It is nowadays a widely used tool for the analysis of nano-scale semiconductor devices, the physical dimensions of which are forever decreasing. The KPFM technique consists of applying a DC bias in order to minimise the electrostatic force between a sample and the scanning tip. From this DC bias, the surface potential of the sample can be deduced relative to the known work-function of the tip. The surface potential strongly depends on surface properties, such as the surface degradation after exposure to air and might depend as well on the nature of the shallow interfaces between semiconductors with different physical properties. Therefore, KPFM allows a contactless and non-destructive electrical or even optical characterization of interfaces in the dark or under illumination (Kronik 1999). Insitu or ex situ applications of KPFM are useful for process monitoring and quality control of actual structures of nano-sized devices. It is possible to largely save time and money assessing the quality of a layered structure before any irreversible degradation. Recent applications include the identification of potential profiles and the prediction of the ultimate performance of solar cells (Bergmann et al. 2016; Challinger et al. 2017; Chen et al. 2017; Garrett et al. 2017) and lasers (González et al. 2017), the prediction of energy levels (Harwell et al. 2016; Kitaura et al. 2017) and the assessment of heterojunctions (Minj et al. 2016; Singh et al. 2017). In the work, a theoretical model is developed in order to simulate KPFM characterization under steady state conditions and under illumination. The model aims at analysing KPFM experimental results and correlating the interface properties with the optoelectronic device performance. Halide perovskite solar cell (PSC), a hot and promising subject in the field of photovoltaics, is chosen to illustrate the model and paves the way for further investigations of more complicated structures. As far as we know, the theoretical analysis of KPFM under illumination is still in its infancy (Bergmann et al. 2016).

2 Numerical modelling

2.1 Fundamental concepts

Firstly, the Fermi level (E_f) is defined for completeness, as the energy level which has a 50% probability of being occupied by electron at any given time. Electrons being fermions, their energy distribution in conduction and valence bands is described by the Fermi–Dirac distribution, which is characterised by E_f . The difference between vacuum level and E_f is equivalent to so-called work-function (WF) of a material. As shown in Fig. 1, when the tip and the sample with different E_f values are electrically connected at short circuit via an external conductor, and the KPFM tip is placed close to the surface of the sample, the difference in E_f drives a current. Electrons flow from one material to the other along the conductor till the E_f are aligned as a result of this electron redistribution. Correspondingly, the sample surface is positively (or negatively) charged due to losing (or adding) electrons, and an electrostatic force results, according to Coulomb's law. This electrostatic force can be neutralized by applying an external bias between the two materials, thereby injecting charge to exactly reverse the charge flow due to the difference in E_f . The electrostatic force



Fig. 1 Illustration of the basic measurement setup of contact potential difference (CPD). Tip and sample are a separated, b connected at short circuit, c under bias of V_{CPD}

is therefore neutralised when the magnitude of external bias equals to the original E_f difference divided by elementary charge as the following expression.

$$V_{CPD} = \frac{\left(E_{f.tip} - E_{f.sample}\right)}{q} \tag{1}$$

where CPD is the abbreviation of Contact Potential Difference between the tip and sample, and V_{CPD} is the bias neutralising the electrostatic force, and q is the electron charge. As a consequence, the surface potential information of the sample can be deduced from the known WF of the tip. A typical KPFM measurement is conducted in the following way. An AC bias at a given frequency is applied between the tip and the sample in addition to a DC bias. The electrostatic force component at this frequency is proportional to the CPD and it can be nullified by using an electrostatic-force-dependent feedback loop. The sign of the V_{CPD} depends whether the bias is applied to the sample or to the tip. The difference between V_{CPD} in the dark and under illumination is the surface photovoltage (SPV).

2.2 Theoretical approach to KPFM simulation

Previous work (Huang et al. 2017) presents the fundamentals of the simulation of electronic and optical properties of semiconductor device and only the essentials are reviewed in this paper. In order to reproduce KPFM measurements in the dark and under illumination, two simple one dimensional architectures, referring to the experiments (Barnea-Nehoshtan et al. 2014; Gheno et al. 2017) are built using the Silvaco software as shown in Fig. 2. A 10 nm thick insulator-like spacer layer is inserted between the tip and sample surface to ensure the continuity of the potential. The thickness of the spacer is defined by the distance between the tip and the sample surface during KPFM measurements (Gheno et al. 2017). The spacer layer may be air, or vacuum depending on the KPFM setup. In the present study, the material parameters of this spacer layer are the energy band gap (E_g) of



Fig. 2 Schematic representations of the simulated architectures. The scanning tip has a work-function (WF) of 4.8 eV. 'ift' refers to the top interfacial layer, namely the effective surface. 'th' is the thickness, n(p) is the n(p)-type doping level and 'its' is the density of interface trap states. The back of FTO substrate is grounded. An insulator-like spacer layer is inserted between the sample and KPFM tip (see Sect. 2). On the left, the bottom part of TiO₂ (bTiO₂) is heavily doped, while the doping level of the top part of TiO₂ (tTiO₂) is varied. The structure on the right is an extension of that on the left, in which MAPbI₃ perovskite layers are added on top of the structure. The *its* at TiO₂/MAPbI₃ interface and n(TiO₂) are fixed as 10¹⁹ and 5×10^{18} cm⁻³, respectively; tTiO₂ with thicknesses of 240 and 90 nm are separately simulated, referring to a total thickness of 300 and 150 nm, respectively (the structure with th = 240 nm is presented here). The external light shines on the top of MAPbI₃ in the right architecture

12 eV, the electron affinity of zero eV and the vacuum dielectric permittivity ε_0 . The surface is defined as the interface between the spacer layer and the sample. The electric field intensity in the spacer layer is computed to investigate the electrostatic interaction between the tip and the sample, leading to the extraction of the surface WF and E_g in the next sections. In the study, the focus is the static part of electrostatic force without taking the oscillating forces into account, which are necessary to perform topography measurement. The reader can refer to the text book of Sadewasser and Glatzel (Sadewasser and Glatzel 2011) for a more detailed discussion of KPFM measurements in the dark, and to the article by Kronik and Shapira (Kronik 1999) for KPFM measurements under illumination.

3 Results and discussion

3.1 Surface work-function of a TiO₂ slab without surface states

As shown in Fig. 2, F-SnO₂/TiO₂ and F-SnO₂/TiO₂/MAPbI₃ structures are modelled to compute the surface WF of TiO₂ (anatase) with and without interface trap state (ITS) at surface, and extract the E_g from the Surface PhotoVoltage (SPV) induced by photon-generated carriers. On top of the metallic-like heavily fluorine doped SnO₂ substrate (FTO), a layer of heavily n-type doped TiO₂ is necessary to allow intra-band tunnelling and hence efficient electrons transfer through the FTO/TiO₂ interface (Rühle and Cahen 2004;

Snaith and Grätzel 2006). An interfacial TiO_2 layer (ift TiO_2) is used on the top of the structure in the present simulation and its thickness is fixed by comparison to existing experimental data (Dymshits et al. 2015). This thin layer is introduced in order to mimic as simply as possible the effect of the TiO_2 surface roughness.

A computed static band alignment is depicted in Fig. 3, in which the 300 nm thick TiO₂ layer is n-type doped with 5×10^{18} cm⁻³ (Forro et al. 1994; Tang et al. 1994) and free of ITS. An intra-band heterojunction tunnelling model (Silvaco Inc. 2012) is employed at the FTO/TiO₂ interface. Few carriers are present in the insulator-like spacer layer, leading to a uniform electric field. By applying a bias on the tip and grounding the bottom of the FTO layer, the variation of the electrostatic field in the spacer layer is simulated and presented in Fig. 4. The electrostatic field, as well as the electrostatic force, is nullified, when the external bias is 0.6 V, which corresponds to a computed WF of 4.2 eV in reference to the tip WF of 4.8 eV (Palermo et al. 2005). The WF value of 4.2 eV is consistent with the difference between the vacuum level and the E_f in the heavily doped TiO₂ layer.

3.2 Surface work-function of a TiO₂ slab with surface states

Unlike the periodic structure of an ideal crystalline semiconductor, the termination of the periodic structure of a semiconductor at interface may form dipoles and/or localized electronic states, which might function like trap states of energy level within the semiconductor bandgap. The formation of these states are typically due to dangling bonds; interface reconstruction or relaxation by a change in the position and/or chemical bonding configuration; steps and kinks or external atoms captured on the surface, and so on. The surface WF of heavily n-doped TiO₂ measured by KPFM (Gheno et al. 2017) can be as high as 4.5 eV on the top of FTO, while 5.2 eV is obtained on top of glass, for a rather low doping level. The present work analyses the effect of ITS for that purpose.

The computations with acceptor-like trap states on the TiO₂ surface are summarized in Fig. 5a, while no significant change is observed in the case of donor-like ITS. TiO₂ layer of 50 nm in the vicinity of FTO remains high doping level of 5×10^{18} cm⁻³ for tunnelling (Forro et al. 1994), while the doping level of the top part of TiO₂ and the surface trap state density are varied from 5×10^{17} to 10^{19} cm⁻³. The trap level is 1 eV below the conduction band and the capture cross section is 8.3×10^{13} cm² (Miyagi et al. 2001). A high density of



Fig. 3 Static band diagram of the FTO/TiO₂ structure. The band structure in the vicinity of the spacer layer is zoomed out on the right, in which the surface of TiO₂ is free of trap state and the tip locates on the rightmost. The n-type doping level of TiO₂ layer is set to 5×10^{18} cm⁻³



surface states and low doping level of bulk material could result in WF variation as large as 0.8 eV. The experiment-consistent WF of 4.5 eV can be reproduced when $n(\text{TiO}_2)$ and its (TiO_2) equal 5E18 and 1E19 cm⁻³, respectively, and the relative static band alignment is presented in Fig. 5b. The carrier redistribution near the free surface results in a space charge region, and similar phenomenon could be found at the same position in Fig. 3 but with rather low extent. Generally, a high density of active ITS is harmful for optoelectronic devices (Ono and Qi 2016) even in the case of good bulk material quality, while the present work suggests that the combination of KPFM measurement and theoretical computation might be an efficient way to quantitatively study this issue and further improve device performance.

3.3 Surface photovoltage in a perovskite hetero-structure on TiO₂

The analysis of V_{CPD} changes induced by illumination can afford quantitative characterization of the bandgap, the doping type, the carrier diffusion length and lifetime, and even energy levels in quantum structures and carrier accumulation in thin film structures (Kronik and Shapira 2001). Since the pioneering work of Brattain and Bardeen in the early 1950s (Brattain and Bardeen 1953), the description of surface photovoltaic phenomena has



Fig. 5 (Color online) **a** Static contact potential difference (CPD.Dark) and work-function as a function of the doping level, $n(tTiO_2)$ and the surface trap density, its(TiO_2). **b** Schematic of static band alignment with acceptor-like trap states of 10^{19} cm⁻³ on the top of 5 × 10^{18} cm⁻³ doped TiO₂

evolved considerably from the fundamental viewpoint while strong progresses have been made for surface and bulk experimental characterizations.

As shown on the right of Fig. 2, a structure FTO/TIO₂/MAPbI₃ is modelled to investigate SPV in this section. The results of the present theoretical study are compared to the experimental SPV results, which were obtained on MAPbI3-xClx mixed halide perovskites (Barnea-Nehoshtan et al. 2014). It is shown in the literature that the Cl content in these alloys is very low and that the chlorine atoms are essentially located in the final structures at the interfaces (Colella et al. 2013). Cl atoms are essentially useful for the initial nucleation of the perovskite seeds in the precursors solution and to enhance the crystallinity of the final perovskite films (Tsai et al. 2017). We thus consider the absorption spectrum and the band structure of bulk MAPbI₃ (Ball et al. 2015). The electronic bandgap deduced in the experimental study on SPV (Barnea-Nehoshtan et al. 2014) is indeed the same as bulk MAPbI₃. TiO₂ layers with thicknesses of 300 and 150 nm are simulated in this section (Fig. 2). MAPbI₃ layers with different thicknesses are deposited on the top of the TiO₂ layer. The MAPbI₃ layers are lightly p doped (Aharon et al. 2014; Jiang et al. 2015) and donor-like surface trap states of 10^{16} cm⁻³ are introduced (Yang et al. 2015). The trap level is located at 0.6 eV above the valence band maximum (Levine et al. 2016), and trap states of 1E19 cm⁻³ are introduced at the TiO₂/MAPbI₃ interface. The simulated band alignment under illumination is presented in Fig. 6a, in which the external light illuminates a 200 nm MAPbI₃layer from the top. Due to the light absorption, E_f is split into two quasi fermi levels of electron (nE_f) and hole (pE_f) , separately. The related carrier distributions are represented in Fig. 6b. Driven by the build-in electric field of the p-n junction, the photon-generated electrons and holes are separated and shifted to the different regions; Holes accumulate near the free surface, and electrons are driven to the other side. However, due to the high density of trap states at the TiO₂/MAPbI₃ interface, a fraction of the electrons are captured in the vicinity of this interface, where a part of the holes are unexpectedly accumulated as well. The detrimental effect of trap states at the TiO₂/ MAPbI₃ interface is deleterious for photon-generated carrier collection and can directly



Fig. 6 (Color online) **a** Band diagram of FTO/TiO₂/MAPbI₃ structure under one sun illumination. On the top of 5×10^{18} cm⁻³ doped TiO₂, the slightly p-doped MAPbI₃ is covered by donor like surface states of 10^{16} cm⁻³. The external one sun shines on the top of MAPbI₃. **b** Carrier distributions in static condition and under illumination. Due to the interface trap states, the reduction of the electron density at the TiO₂/MAPbI₃ interface is observed in the dark (black squares) and under illumination (green triangles). The accumulations of photon-generated hole (red circles) are observed at the TiO₂/MAPbI₃ and MAPbI₃/spacer interfaces. However, in the dark, the hole density in the depleted MAPbI₃ is too low to be represented with the same scale



Fig. 7 a Experimental and simulated results of surface photovoltage spectroscopy (SPS). The simulated light power is 1 W/cm². The results of the computation for two thicknesses of TiO_2 are compared. **b** Computed surface work-function and surface photo voltage (SPV) as a function of the thickness of the MAPbI₃ layer. The external light source corresponds to one sun

decrease solar cell efficiency (Zhou et al. 2014). Under illumination, the carrier redistribution results in a variation of V_{CPD} , and the difference between V_{CPD} in the dark and under illumination is named as the SPV. For example, the V_{CPD} of the structure in Fig. 6 under one sun illumination equals to 0.603 V and the V_{CPD} in the dark is 0.275 V, leading to a SPV of 0.328 V.

In addition, the Surface Photovoltage (SPV) is computed in comparison with experimental data obtained by Surface Photovoltage Spectroscopy (SPS) (Barnea-Nehoshtan et al. 2014), as shown in Fig. 7a. The energy bandgap of MAPbI₃ around 1.55 eV is deduced from the SPV edge and consistent with the absorption spectrum (Lin et al. 2014). No significant differences are observed from the computation of the SPV edge with different thicknesses of the TiO₂ layer. Furthermore, the SPV is calculated as a function of the thickness of the MAPbI₃ layer and presented in Fig. 7b. When the intrinsic MAPbI₃ is thinner than 100 nm, the surface WF is closed to the surface WF of the underneath TiO₂ layer (4.5 eV). The surface WF increases up to 5.06 eV, when the thickness of MAPbI₃ layer and presented in Fig. 7iO₂ layer is screened by thick MAPbI₃ layers. When the MAPbI₃ layer thickness increases, the V_{CPD} under light is found to be almost constant due to a certain amount of photon-generated holes accumulated at the free surface. However, the V_{CPD} in the dark, namely WF progressively decreases till saturation, leads in turn to a variation of SPV.

3.4 Conclusions

A new approach to modelling Kelvin Probe Force Microscopy for hetero-structures in the dark and under illumination has been presented. The approach has been tested by examining FTO/TiO_2 and $FTO/TiO_2/MAPbI_3$ structures. Unexpected surface states on the top of TiO_2 layer are inferred by the comparison of a theoretical computation and experimental results. The basic applications of KPFM under illumination are analysed as well. Due to its sensitivity to the surface conditions, to photon-generated charges and to shallow interfaces, the KPFM characterization technique might be helpful to monitor the fabrication of planar

hetero-structures and devices. Further study on more complicated structures, such as quantum structures or cross sections is underway.

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