NUMERICAL ANALYSIS OF KELVIN PROBE FORCE MICROSCOPY

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Abstract

Kelvin probe force microscopy (KPFM) is an advanced local characterisation technique which allows nanometric scale characterisation. It consists of placing a scanning metallic tip near a sample surface and varying the bias applied between the two so as to minimise the electrostatic force on the probe, yielding the contact potential. The technique can be extended to light and dark conditions, and a range of methods employed to minimise the force. Scanning as a function of position can yield information on carrier transport properties and on the band structure of materials as a function of composition on a local scale. This includes local lifetime measurement, band profiling including workfunction, and interface characterisation including defect properties. This provides a multiscale link between properties on the local scale and the device scale. The technique however is difficult to interpret since it is inherently a surface probe, and as such is determined by surface properties and in particular by surface defects. It is therefore necessary to apply modelling techniques to enable the interpretation of characterisation in order to extract useful information on bulk properties.

This work presents results on numerical modelling of this technique using in-house software interfaced with Silvaco numerical modelling in order to interpret experimental KPFM characterisation.

The model includes acceptor and donor defect layers at the surface or extending into the volume of the sample, and both dark and arbitrary illuminated measurements. The model evaluates the field directly sensed by the probe between the tip and the sample surface, and also evaluates the field in the volume of the sample in order to bridge gap between the surface measurement and the bulk proprties. The first yields the minimum force as measured by the tip, whereas the second provides band profiles and charge densities in the volume of the sample, enabling the experimental characterisation to be linked to the bulk properties.

The application of the model to homogeneous and inhomogeneous structures is presented in the light and in the dark, enabling information on the precise nature of KPFM measurement and the origin of the contact potential difference to be analysed as a function of minority as well as majority carrier densities. The effect of defect states and their distribution in energy and within the sample volume is discussed. Experimental characterisation results are presented and analysed in terms of this model.

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