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Simulation of the capacitance-voltage characteristic in the case of epitaxial ferroelectric films with Schottky contacts

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ABSTRACT

The current–voltage (*C-V*) characteristic of epitaxial ferroelectric films is simulated assuming the presence of Schottky-type contacts at the two electrode interfaces. The model assumes that the overall capacitance of the metal-ferroelectric-metal (*MFM*) structure is composed of two parts: (i) one associated with the Schottky contacts, in which the ferroelectric polarization is saturated, the dielectric constant is independent on the voltage and only the linear response to the applied electric field is taken into account; (ii) one related to the ferroelectric volume, where the dielectric constant is voltage dependent through the hysteresis response of the ferroelectric polarization. The most important result of the model is that it can simulate the experimentally observed thickness dependence of the dielectric constant without considering a so-called "dead layer" at the electrode interface. The model renders *C-V* characteristics in good qualitative agreement with the experimental ones in the case of an *MFM* structure based on epitaxial *PZT* films. The quantitative fit suggests that the behaviour of the ferroelectric polarization during the *C-V* measurement may be very different from its behaviour during the hysteresis measurement. This is explained by the fact that the two measurements have very different principles. It is also found that the dielectric constant of the ferroelectric volume has a different voltage dependence compared to the one derived from the hysteresis loop or from the experimental *C-V* characteristic. This is also related to the different measurement principles and to the fact that the measured capacitance of the *MFM* structure includes, besides the ferroelectric volume, the voltage dependent capacitance of the Schottky contacts.

1. Introduction

One of the most basic characterization methods for metal–semiconductor Schottky contacts (or diodes), semiconductor p-n junctions or metal-oxide-semiconductor (*MOS*) structures, is the capacitance–voltage (*C-V*) measurement [1], [2]. The obtained *C-V* characteristic can be used to extract important information such as: doping concentration, doping profile, build-in potential, flat band voltage, oxide capacitance (for *MOS* structures), density of interface states, charge density in the oxide layer, etc. [2]. For ferroelectric-based structures such as metal-ferroelectric-semiconductor (*MFS*) or metal-ferroelectric-metal (*MFM*), the same basic measurement is usually employed. It is well known that the butterfly shape of the *C-V* characteristic for a ferroelectric capacitor is a fingerprint for the presence of ferroelectricity, while the hysteresis observed in the *C-V* characteristics of a *MFS* structure is important for non-volatile memories and for ferroelectric field effect transistors [3], [4], [5], [6].

There are a number of theoretical models developed to simulate the *C-V* characteristics for *MFS* structures and variants like metal-ferroelectric-insulator-semiconductor structures (*MFIS*) [7], [8], [9]. The theoretical models designed for *MFM* structures, however, have been focusing on simulating mainly the hysteresis loop [10], [11], [12], [13] and only some of them were approaching the problem of the *C-V* characteristic [14], [15]. The aim in many cases was to explain the experimentally observed ferroelectric layer thickness dependence of the dielectric constant [16], [17]. In most cases the presence of a so-called "dead layer" near the electrode interface was assumed, with a dielectric constant significantly lower than that of the ferroelectric volume [18], [19], [20], [21]. However, the experimental evidences are both pro and against this hypothesis and thus the matter remains controversial as yet [22], [23], [24], [25]. Adding to the controversy, experimental results reported in the literature also indicate the presence of Schottky type contacts at the electrode interfaces in *MFM* structures [26], [27], [28], [29], [30] which should be factored into theoretical models attempting to simulate their electrical properties. Therefore, attempts were performed to include Schottky contacts in models designed to analyse and simulate the frequency dependence of capacitance or the voltage dependence of the leakage current [26], [31], [32], [33].

The present paper continues the effort to develop coherent models for simulating the electrical properties of *MFM* structures based on

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epitaxial ferroelectric films by accounting for the Schottky-type contacts in modelling the *C-V* characteristic and of the thickness dependence of the dielectric constant. Although the Schottky contacts are often considered in analysing the experimental *C-V* characteristics [34], [35], [36], [37] simulations based on equivalent circuits similar to the ones used to explain the frequency dependence of capacitance are lacking. Here we show that the *C-V* characteristics simulated by using such circuits are in good qualitative agreement with the experimental one. The thickness dependence of the dielectric constant can also be simulated without any need for including the so-called "dead layers" assumption at the electrode interfaces. However, the quantitative fit of the simulated and experimental *C-V* characteristics is possible only by assuming a different magnitude of the remnant polarization compared to the one extracted from the experimental hysteresis loop. This is discussed considering the basic differences between the measurement principles of the two experimental techniques, which can lead to different behaviours of polarization under the applied electric field. It is also found that the voltage dependence of the dielectric constant associated with the ferroelectric volume of the *MFM* structure, as resulting from the model, is very different from the one derived from the hysteresis loop or from the experimental *C-V* characteristic. These aspects are also discussed in the paper, underlying the differences between theoretical models and usual experimental interpretations.

2. Theoretical model

As suggested by the previous approaches developed to analyse and simulate the electrical properties of *MFM* structures based on epitaxial films, the equivalent circuit used to model the *C-V* characteristic should include the two back-to-back Schottky contacts/diodes associated with the electrode interfaces [16], [17], [31], [32], [33], [34], [35], [37]. Therefore, whatever the polarity of the applied voltage one of the contacts/diodes will be reverse-biased and its voltage dependent capacitance C_i should be considered in calculations. The band diagram for a perfectly symmetric test structure is presented in Fig. 1a, considering an *n-type* ferroelectric semiconductor. The free carrier concentration n is considered equal with the fixed space charge density N_{eff} in the depleted region (the presence of charged traps is neglected). The doping is considered uniform in the film and thus n does not depend on the position. The equivalent circuit associated with the *MFM* structure is presented in Fig. 1b, and consists of three parallel *R-C* groupings connected in series. The left and right groupings represent the two interfaces while the one in the middle represents the ferroelectric volume. The ferroelectric polarization is considered equivalent to the dipole moment of a couple of charged sheets, with equal and opposite charges, each located at a fixed finite distance X_i from the corresponding

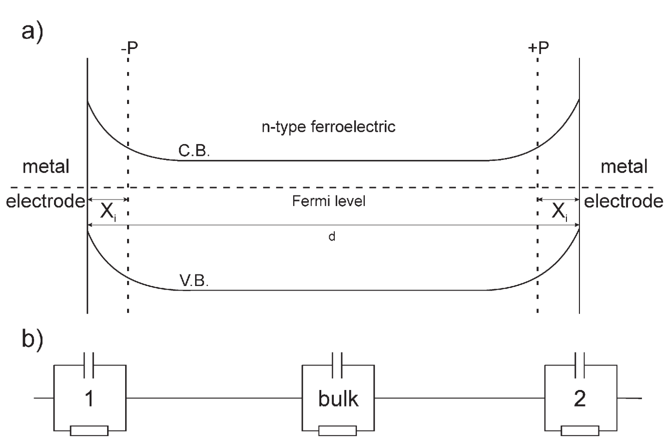

Fig. 1. a) Assumed energy band diagram for the *MFM* structure showing the two charged sheets in the vicinity of the interfaces and b) equivalent circuit used to characterize the *MFM* structure.

physical metal-ferroelectric interface ($i = 1,2$ for the two electrode interfaces). One has to mention that these are not "dead layers" but should be regarded as domains in which the polarization drops from its maximum value in the ferroelectric volume to zero at the physical electrode interfaces [36], [38], [39].

It was shown in a previous paper that the polarization charges produce a strong influence on the built-in potential V_{bi} [31], [32]. Thus the new built-in potential V'_{bi} can be written as:

$$V'_{bi} = V_{bi} \mp \frac{P_s}{\varepsilon_0 \, \varepsilon_{st}} X_i, \tag{1}$$

where, P_s is the saturated ferroelectric polarization [40], ε_0 is the vacuum dielectric permittivity, ε_{st} is the static dielectric constant of the ferroelectric and X_i is the thickness of the interface layer. The (-) sign is valid when the polarization charge is of the same sign with the fixed charges in the depleted region (positive for an *n-type* semiconductor). The (+) in Eq. (1) is valid when the polarization and fixed charges in the depletion region have opposite signs.

The capacitance C_i of the Schottky contacts at the electrode-ferroelectric interfaces will be given by the same equation used for metal–semiconductor contacts only that V_{bi} is replaced with V'_{bi}:

$$C_i = \frac{\varepsilon_0 \, \varepsilon_{st}}{w_i} = A \sqrt{\frac{q \, N_{eff} \, \varepsilon_0 \, \varepsilon_{st}}{2\left(V + V'_{bi} - \frac{k_B \, T}{q}\right)}}. \tag{2}$$

The notations are as follows: w_i — width of the depletion region; q — electron charge; V — applied dc voltage; k_B — Boltzmann's constant; T — system temperature. In the following discussion the term $k_B \, T/q$ in Eq. (2) will be neglected. However, in the *C-V* measurement the capacitance at a certain *dc* voltage is measured by superimposing a small amplitude *ac* voltage. In fact, the *dc* voltage only sets the polarization state. The actual capacitance measurement of the *MFM* structure is performed with the small *ac* voltage. Therefore, the capacitance is extracted from an *ac* measurement and the entire structure should be regarded as an impedance. The total impedance of the equivalent circuit presented in Fig. 1b will be:

$$Z_t = \left(\frac{1}{R_b} + j\omega C_b\right)^{-1} + \sum_{i=1,2}\left(\frac{1}{R_i} + j\omega C_i\right)^{-1}, \tag{3}$$

where, the index b refers to the bulk of the film (the so-called neutral volume in case of semiconductors), i refers to one of the two interfaces ($i = 1,2$) and $\omega = 2\,\pi\, f$, f being the frequency of the small *ac* signal. The interfaces are usually not identical, even when the top and the bottom electrodes are from the same metal. The different processing and thermal histories can induce differences in the top and bottom interface properties. However, in order to simplify the simulations, we will assume identical interfaces in the present case.

A simplifying assumption for the *MFM* case is that the resistance of the depleted regions is very high. Thus, the depleted regions act as pure capacitances, given by Eq. (2) with V_{bi} replaced by V'_{bi} (given by Eq. (1)). Only the capacitance of the reverse-biased contact will be considered in the following computation. The capacitance of the forward biased contact is considered to increase very fast with the voltage, so that the corresponding capacitance becomes negligible compared to the one of the reverse-biased contact. The dielectric constant used in Eqs. (1) and (2) is assumed to include only the linear part of the dielectric response (the non-switching contribution), without any contribution from the non-linear ferroelectric polarization [40]. In other words it is assumed that in the depleted region associated with the Schottky contact the dielectric constant is voltage independent and that the ferroelectric polarization is saturated by the internal electric field present at the interface [36], [40]. The dielectric constant