Study of ferroelectric and elastic properties of ferroelectric capacitors based on hafnium oxide films by Band Excitation techniques

M. Spiridonov, S. Zakharchenko, A. Chouprik, A. Chernikova, R. Kirtaev, D. Negrov

[1]*Moscow Institute of Physics and Technology, Dolgoprudny, 141700, Russia*
e-mail: spiridonob@yandex.ru

The Band Excitation (BE) approach [1,2] in piezoresponse force microscopy (PFM) provides an alternative to standard single frequency PFM technique by exciting and detecting response at all frequencies within a specified frequency range simultaneously. BE introduces a synthesized digital signal that spans a continuous band of frequencies, and monitors the response within the same frequency band. This approach allows to obtain full piezo- and mecanical response spectra and process them considering the specific conditions like atomic force microscopy (AFM) background. Resonance-enhanced combined band-excitation (BE) PFM and atomic force acoustic microscopy (BE AFAM) techniques was home-implemented [3] in commercially available AFM Ntegra (NT-MDT) using digital signal processor (Nanoscan Technologies) to study domain structure of ferroelectric (FE) thin $Hf_{0.5}Zr_{0.5}O_2$ films which are considered as the main functional material for nonvolatile FE random access memory (FeRAM) [4]. Analysis of the local FE and elastic properties of $Hf_{0.5}Zr_{0.5}O_2$ films allows to understand the nature of structural transformations during first stages of FE capacitor operation and paves way to engineering of hafnium oxide memory cells to improve their performance.

For fitting of acquired spectral response, we used the model of harmonic oscillator with additional shift linearly dependent on frequency. The last contribution is intended to compensate a possible AFM background and finally allows to obtain most correct values of piezoresponse amplitude and phase. For fitting, we applied the vector technique [5]. Both piezo- and mechanical contact response was fitted with the rational function approximation $H(s) = \frac{c_0}{s-a_0} - \frac{c_0}{s-\bar{a}_0} + d + sh$, where s is complex frequency parameter, a_0 and $\bar{a}_0$ are two complex conjugate poles, c_0 is residue, d is shift parameter, h is slope parameter. First two factors in transfer function $H(s)$ represent resonant system formed by cantilever in contact with sample surface, while the expression $d + sh$ describes AFM background in AFM Ntegra. Both in BE PFM and BE AFAM, in each point of scan the optimal parameters of the fit yield resonance amplitude A, phase φ, contact resonance frequency f_c, d and h parameters in each point of scan. In addition, we calculate parameter Q, typically characterizes quality factor. Therefore, 12 parameters are mapped during scanning in PFM and AFAM: A, φ, f_c, Q, d h . Obtained data contains a diversity of information about the FE and elastic properties of structure under investigation. In addition to domain structure, the local elastic properties (including Young's modulus, parameter of dissipation, mechanical stress) can be acquired and analyzed. In addition, the information about mechanical response allows to eliminate the topographical crosstalk in PFM data.

In conclusion, the combined band-excitation BE PFM and BE AFAM technique allows to reveal the domain structure of novel FE thin $Hf_{0.5}Zr_{0.5}O_2$ films and obtain the additional information about evolution of elastic properties during the operation of memory cell.

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