Positron Annihilation Spectroscopy: An Emerging Technique For Characterization of Oxygen Vacancies in Hf-based-high-K Materials?

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Introduction

High-K metal gate (HMGK) stacks required to tackle the technological issues brought by the drastic reduction of gate length of CMOS devices (nodes < 32 nm). Use of high-K dielectrics (HfO2) and metal gate (TaN) induces shifts in transistor Vt, assumed to be related to oxygen vacancies [VΩ] in both HfO2 and SiO2.

To assess these mechanisms, characterization of VΩ by two techniques:
- Positron annihilation spectroscopy (PAS): the most sensitive characterization method to vacancies
- Electron energy loss spectroscopy (EELS): potentially sensitive to VΩ, spatial resolution compatible with HfMGK structures.

PAS used to characterize vacancies in diverse materials.10, 11, 12, 13 but only few studies for high-K.8, 10, 11

Experimental

Positron emission: 3β radioactive source 22Na
Moderator (mosoiconic beam converter): 5 μm thick tungsten foil
Accelerator: Kinetik energy 0.2 to 25 keV
Flux: 10^10 cm^-2
Detector: high purity Ge, resolution 1.1 keV at 511 keV, efficiency >25% at 1.33 MeV

Measurement of (e+, e) pair momentum distribution by recording the Doppler broadening of the 511 keV annihilation line (ΔE).

Extraction of low and high W momentum annihilation fraction in respectively the momentum windows [0 ... 2.80 (10±50)] and [10.61 ... 26.35] 10^50 m^-1 where m is the mass of the electron and c, the speed of light.

5 W annihilations with low momentum electrons, valence electrons
W annihilations with high momentum electrons, core electrons
5 W and extracted at energies ranging from 0.2 to 25 keV with step increasing from 0.2 to 1 keV

Results and discussion

PAS - Implantation profile

P(0): probability of positron implantation for each energy
Mean depth implantation: z_m = 0.88z_2
P(z) = 1 - (3.86 z / z_m)

E: Positron energy μJ: material density A, m and μ are material dependent constants (p. 33 ref. 12)

PAS - VEPFIT simulation

VEPFIT, fit and mediation software for PAS:
- Taking account of implantation profile and diffusion
- Sample divided into several homogeneous layers
- S, W parameters determined in each layer and added, after taking account of implantation probability, to give the total S and W
- Determination of other parameters such as effective diffusion lengths

Simulation scheme:
- 50 nm thick HfO2 layer on Si
- Measured annihilation parameters for Si substrate, with l, the diffusion length.
- Interfacial layer with electronic field ranging from 37 to 10^5 keV/μm

As deposited (PAS)

As deposited vs annealing (PAS, 50 nm thick layers)
After annealing: Si characteristics reached more quickly, energy range governed by annihilation in HfO2, narrowed. S, W parameters:
- Defect concentration increases during annealing in HfO2/Si interface.
- Positively charged defects at HfO2/Si interface.

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References