

ATOMISTIC MODELING OF METAL/HIGH-K OXIDE INTERFACE PROPERTIES AS FUNCTION OF GAS TREATMENT

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The depletion length in the current polysilicon gate technology increases the effective oxide thickness and thus reduces the advantages of using high-k dielectrics in the future generations of CMOS technology. Moreover, it was recognized that new high-k materials can react with the polySi gate causing undesirable changes in the electrical properties. All these problems can be solved by using a combination of a high-k ceramics with a suitable metal gate as a replacement for SiO₂ and polySi. In this work we considered dependence of metal / high-k oxide interface properties on the gas treatment conditions.

We present an atomistic investigation of the structure and properties of the interfaces between metal and high-k oxide materials, considering as an example metal/HfO₂ interface.

The dependence of Pt/HfO₂ interface structures and properties (the adhesion and the band offset at the interface) on the interfacial oxygen concentration is determined (see Fig. 1). Using calculated energies for series of structures with different interfacial oxygen concentration we predicted equilibrium interface structure dependence on partial pressure of oxygen and temperature. The predicted oxygen-pressure dependence of the interface composition provides a satisfactory explanation of the known dependence [1] of electrical properties on the gate deposition conditions (see Fig. 2).

It is also shown by calculated results that oxygen chemical potential strongly influences on the segregation trends at the oxide/metal alloy interface, in particular, for the Mo–Pt/HfO₂ interface large oxygen chemical potential leads to Mo segregation to the interface.

The possibility of tuning electrical properties by interface doping with impurity atoms such as N, F, or Cl is discussed. We found that N doping of the Pt/HfO₂ interface is unstable with respect to thermodynamics of desorption to gas phase, while doping with Cl is thermoneutral and doping with F atoms is exothermic. F atoms at the Pt/HfO₂ results in increasing of valence band offset at the interface with respect to oxygen-free Pt/HfO₂ interface. Doping of Mo/HfO₂ interface with nitrogen is stable with respect to nitrogen desorption to gas phase and results in increasing of effective work function of Mo.

References:

[1] J.K. Schaeffer, L.R.C Fonseca, S.B. Samavedam, Y. Liang, P.J. Tobin, and B.E. White, Appl. Phys. Lett., **85** (2004) 1826.

Figures:

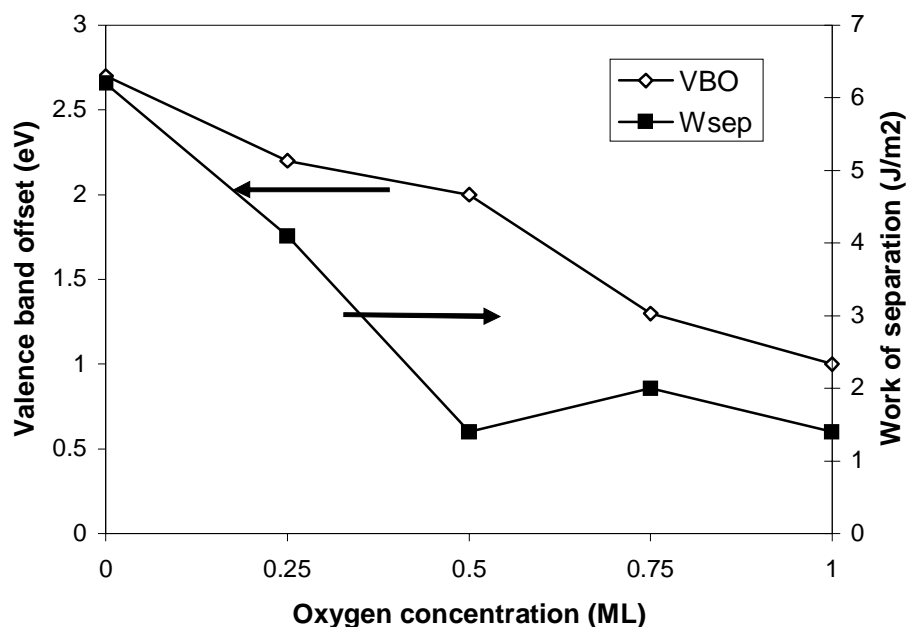


Fig. 1. Calculated valence band offset (VBO) and work of separation (W_{sep}) for the Pt/HfO₂ interface as a function of interfacial oxygen concentration.

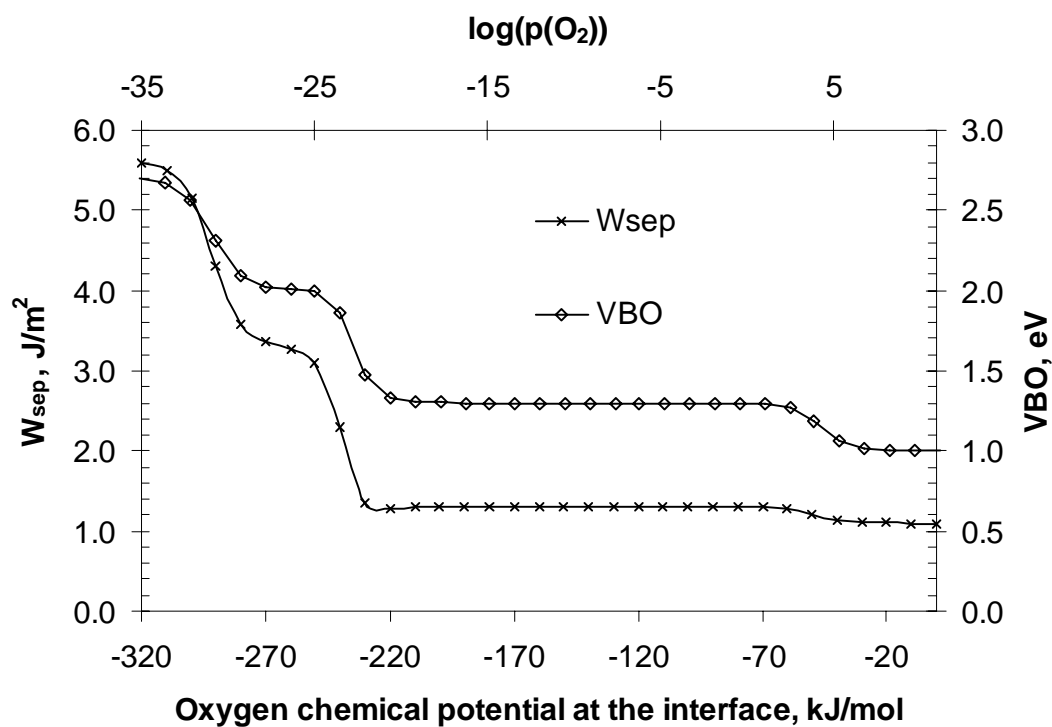


Fig. 2. Work of separation and valence band offset (VBO) for the Pt/HfO₂ interface as a function of the oxygen chemical potential at 500°C.