Electronic Supplementary Information for:

Atomic Layer Deposition of B_2O_3/SiO_2 Thin Films and Their Application in an Efficient Diffusion Doping Process

Woo-Hee Kim,[a,b] Il-Kwon Oh,[a] Min-Kyu Kim,[a] Wan Joo Maeng,[a] Chang-Wan Lee,[a] Gyeongho Lee,[a] Clement Lansalot-Matras,[c] Wontae Noh,[c] David Thompson,[d] David Chu[d] and Hyungjun Kim[a,*]

[a] School of Electrical and Electronic Engineering, Yonsei University, 262 Seongsanno, Seodaemun-gu, Seoul 120-749, Korea

[b] Department of Chemical Engineering, Stanford University, 381 North-South Mall, Stanford, California 94305, United States

[c] Air Liquide Korea Co., Yonsei University, 50 Yonsei-Ro, Seodaemun-Gu, Seoul 120-749, Republic of Korea

[d] Applied Materials, 974 E. Arques Avenue, M/S 81280, Sunnyvale, California 94085, United States

*Authors to whom correspondence should be addressed.

E-mail: hyungjun@yonsei.ac.kr. Telephone: +82-2-2123-5773; Fax: +82-2-313-2879.

(1) Precursor information used in this study

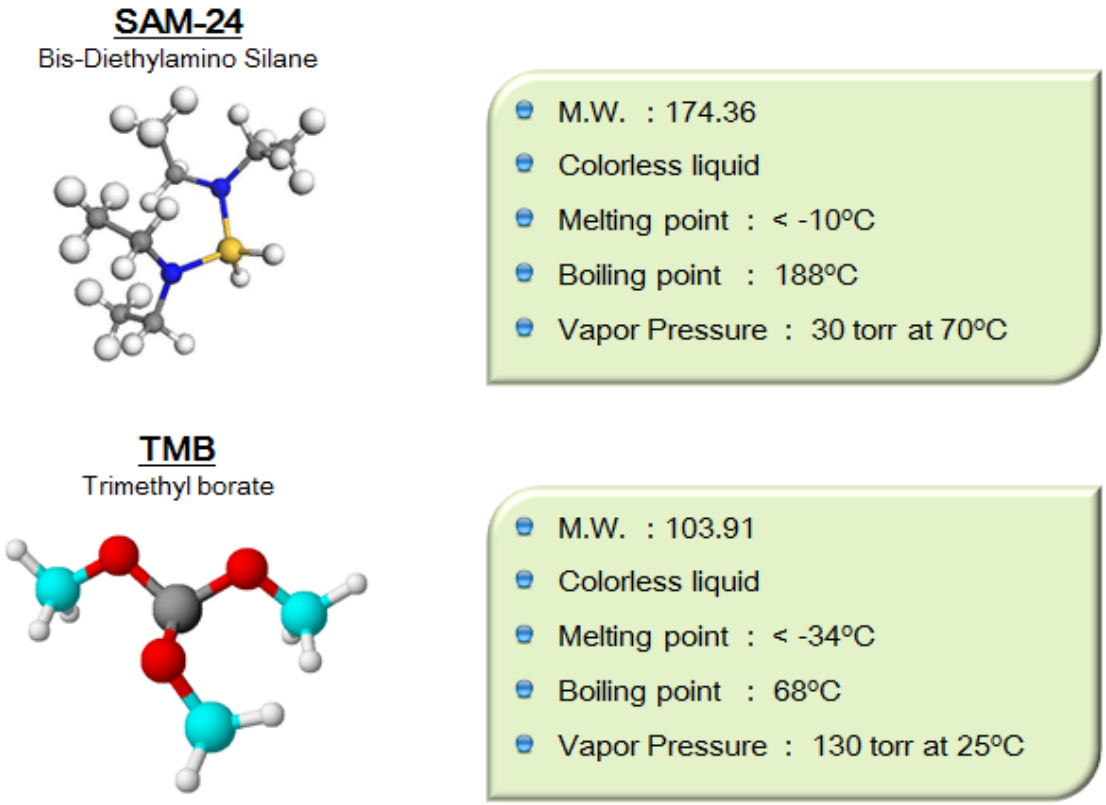

Figure S1. Detailed precursor information for ALD of SiO_2 (upper part) and B_2O_3 (lower part).

(2) Conformality of ALD SiO_2 film in a via hole structure

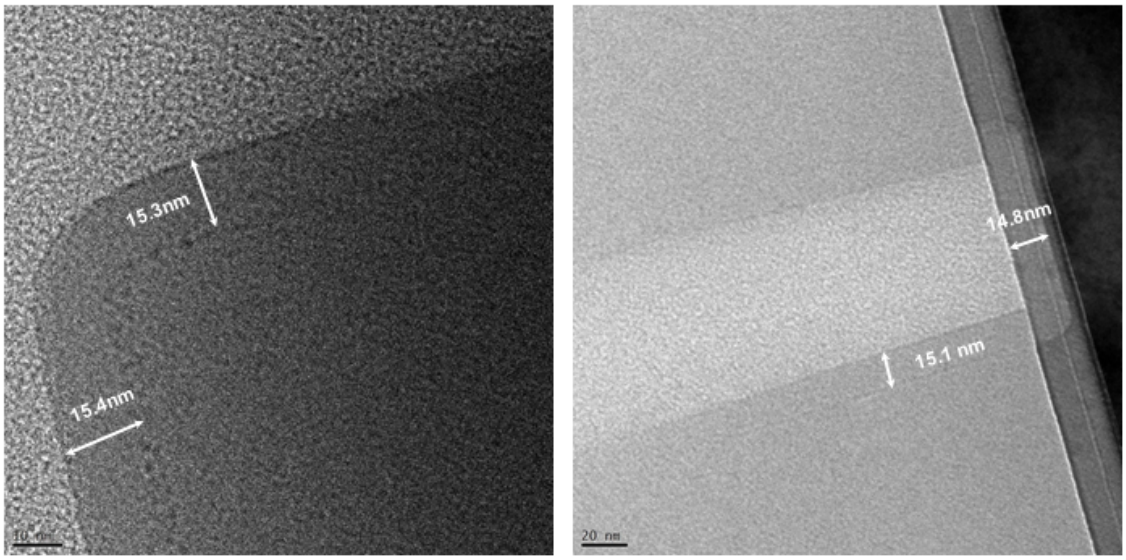

Figure S2. Cross-sectional transmission electron microscopy (X-TEM) images for 15 nm-thick ALD SiO_2 film deposited by using SAM-24 and O_2 plasma in a nanoscale via hole (aspect ratio of 5:1).

(3) Formation of interface dipole layers by oxygen areal density model[1)]

Table S1. Summary of structural parameters of SiO_2 and B_2O_3, including density, volume of unit structure containing one oxygen atom (V_u), and normalized areal oxygen density (σ/σ_{SiO2}).

Oxides	SiO_2	B_2O_3
Density (g/cm^3)	2.2	2.55(Trigonal)/3.11(Monoclinic)
Unit structure	$Si_{1/2}O$	$B_{2/3}O$
V_u ($Å^3$)	22.7	15.1(Trigonal)/12.4(Monoclinic)
σ/σ_{SiO2}	1.00	1.31(Trigonal)/1.49(Monoclinic)

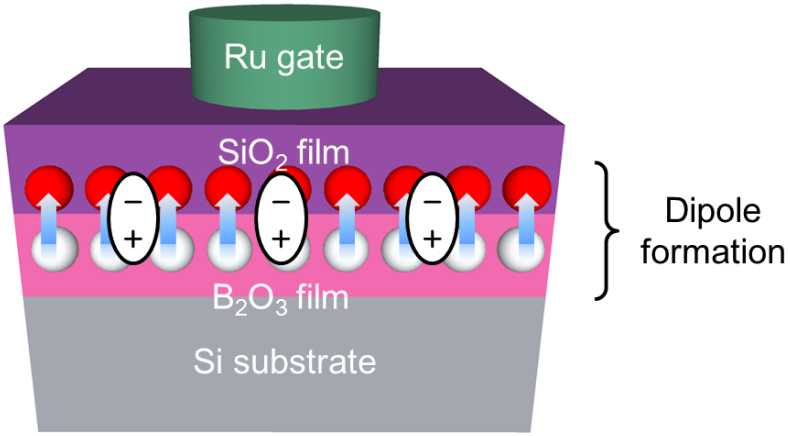

Figure S3. Schematic of the formation of interface dipole layers due to the oxygen transfer, in the form of negatively charged ion, creating the positively charged oxygen vacancies in higher σ oxide region, and negatively charged center in lower σ oxide region.

(4) Preparation of B-doped SiO_2 films with different B/(B+Si) composition

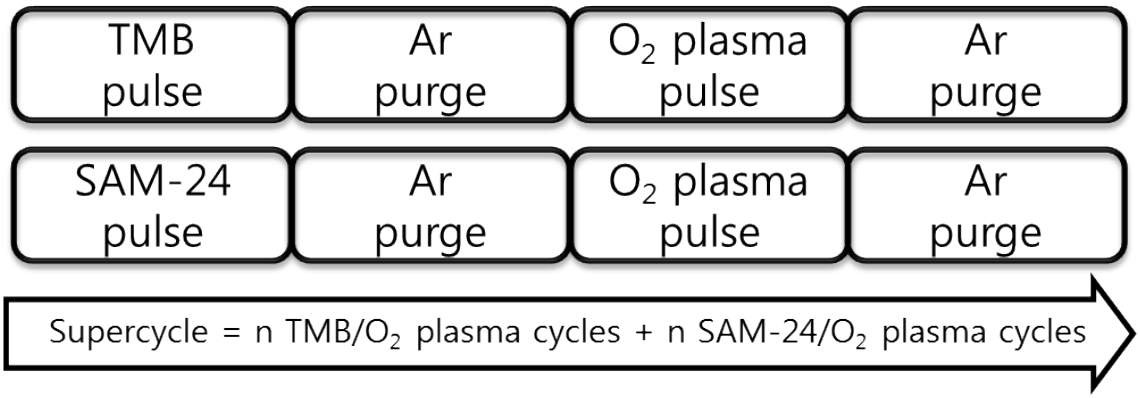

Figure S4. Schematic of the atomic layer deposition (ALD) supercycle, composed of n repetitions of alternating B_2O_3 and SiO_2 growth cycles.

Reference

(1) Kita, K.; Toriumi, A., Origin of electric dipoles formed at high-k/SiO_2 interface. *Appl. Phys. Lett.* **2009,** *94*, 132902-132902-3.