Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Microstructures and electronic characters of β-Ga_2O_3 on different substrates: Exploring the role of surface chemistry and structure

Naxin Zhu [a], Xiangyi Xue [a], Jie Su [a,b*]

[a] State Key Lab of Solidification Processing, College of Materials Science and Engineering, Northwestern Polytechnical University, Xi'an, Shaanxi 710072, PR China

[b] State Key Discipline Laboratory of Wide Band Gap Semiconductor Technology, School of Microelectronics, Xidian University, Xi'an 710071, China

E-mail: sujie@xidian.edu.cn

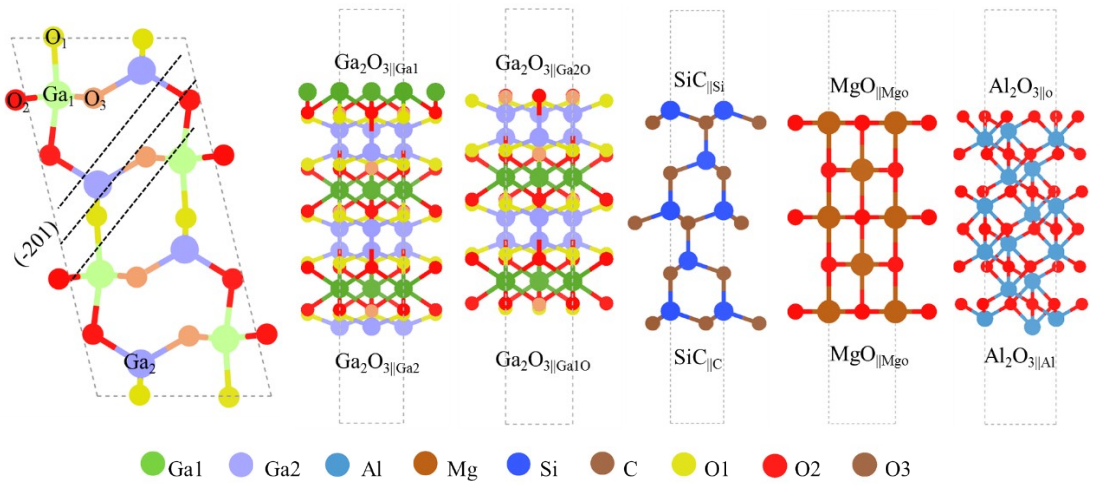

Figure S1. Side views of β-Ga_2O_3, and β-Ga_2O_3 (-201) surfaces, SiC (0001) surfaces, MgO (001) surfaces, Al_2O_3 (001) surfaces with different terminations.

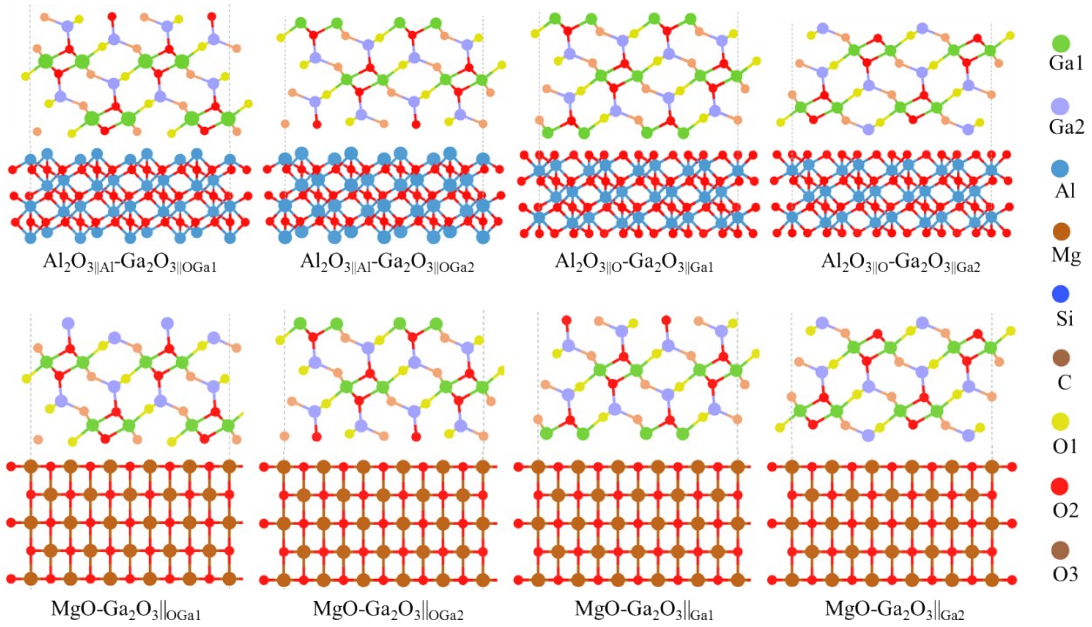

Figure S2. Side views of Al_2O_3-Ga_2O_3 and MgO-Ga_2O_3 interfaces with different terminations.

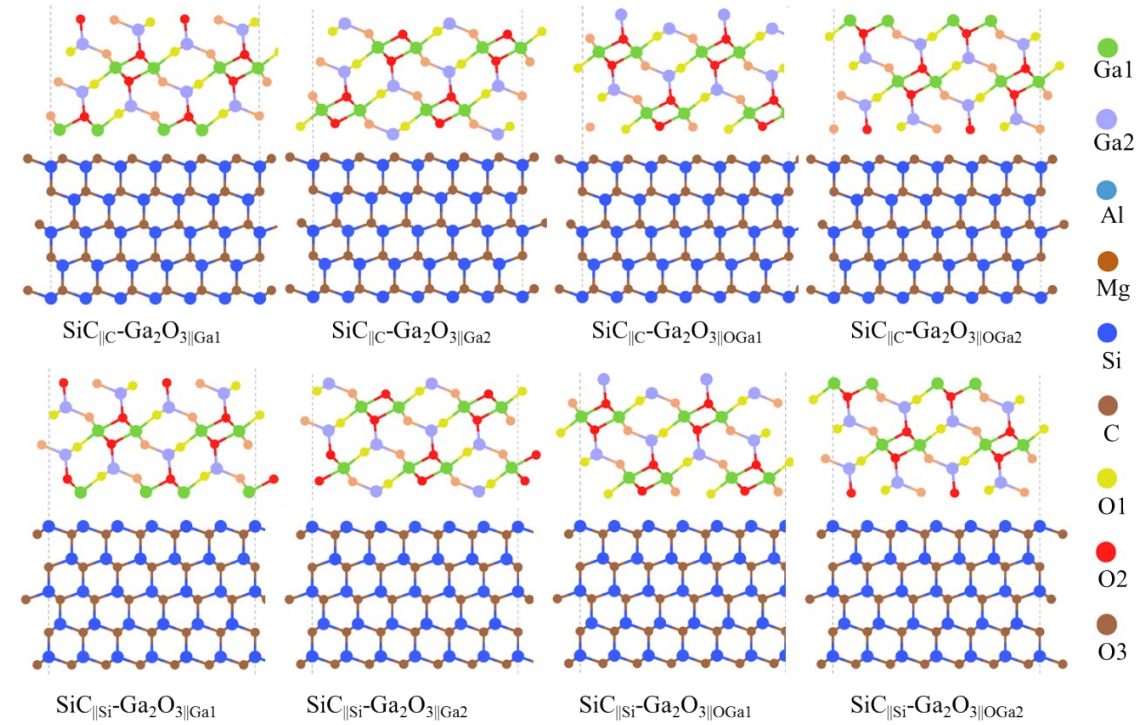

Figure S3. Side views of SiC-Ga_2O_3 interfaces with different terminations.

Table S1. The lattice strain along a and b direction and the average lattice strain of β-Ga_2O_3 in these different Al_2O_3-Ga_2O_3, MgO-Ga_2O_3, and SiC-Ga_2O_3 interfaces. The difference of dangling bonds between Ga_2O_3 and substrate part in these substrate-Ga_2O_3 interfaces with different terminations.

Interface	Strain (%)			Dangling bonds
	a direction	b direction	average	
$Al_2O_{3\|\|Al}$-$Ga_2O_{3\|\|OGa1}$	10.35	2.55	4.3	2
$Al_2O_{3\|\|Al}$-$Ga_2O_{3\|\|OGa2}$	10.35	2.55	4.3	1
$Al_2O_{3\|\|O}$-$Ga_2O_{3\|\|Ga1}$	10.35	2.55	4.3	12
$Al_2O_{3\|\|O}$-$Ga_2O_{3\|\|Ga2}$	10.35	2.55	4.3	12
MgO-$Ga_2O_{3\|\|OGa1}$	-0.34	-3.75	-1.36	8
MgO-$Ga_2O_{3\|\|OGa2}$	-0.34	-3.75	-1.36	8
MgO-$Ga_2O_{3\|\|Ga1}$	-0.34	-3.75	-1.36	2
MgO-$Ga_2O_{3\|\|Ga2}$	-0.34	-3.75	-1.36	5
$SiC_{\|\|C}$-$Ga_2O_{3\|\|OGa1}$	5.73	-1.29	2.52	0
$SiC_{\|\|C}$-$Ga_2O_{3\|\|OGa2}$	5.73	-1.29	2.52	0
$SiC_{\|\|C}$-$Ga_2O_{3\|\|Ga1}$	5.73	-1.29	2.52	2
$SiC_{\|\|C}$-$Ga_2O_{3\|\|Ga2}$	5.73	-1.29	2.52	4
$SiC_{\|\|Si}$-$Ga_2O_{3\|\|OGa1}$	5.73	-1.29	2.52	0
$SiC_{\|\|Si}$-$Ga_2O_{3\|\|OGa2}$	5.73	-1.29	2.52	0
$SiC_{\|\|Si}$-$Ga_2O_{3\|\|Ga1}$	5.73	-1.29	2.52	2
$SiC_{\|\|Si}$-$Ga_2O_{3\|\|Ga2}$	5.73	-1.29	2.52	4

Table S2. The valence band offset (VBO) and conduction band offset (CBO) coupling with the band gap of Ga_2O_3 part in these different Al_2O_3-Ga_2O_3, MgO-Ga_2O_3, and SiC-Ga_2O_3 interfaces.

Interface	VBO (eV)	CBO (eV)	Gap (eV)	Band alignment
$Al_2O_{3\|O}$-$Ga_2O_{3\|Ga2}$	0.02	0.45	2.60	Type-II
$Al_2O_{3\|O}$-$Ga_2O_{3\|Ga1}$	0.10	0.23	2.82	Type-II
$Al_2O_{3\|Al}$-$Ga_2O_{3\|OGa2}$	0.12	0.50	3.30	Type-II
$Al_2O_{3\|Al}$-$Ga_2O_{3\|OGa1}$	0.25	0.94	2.70	Type-II
MgO-$Ga_2O_{3\|Ga2}$	0.12	0.22	3.42	Type-I
MgO-$Ga_2O_{3\|Ga1}$	0.65	0.31	2.79	Type-I
MgO-$Ga_2O_{3\|OGa2}$	0.15	0.58	3.42	Type-I
MgO-$Ga_2O_{3\|OGa1}$	0.25	0.56	3.18	Type-I
$SiC_{\|Si}$-$Ga_2O_{3\|Ga2}$	0.39	0.07	2.43	Type-II
$SiC_{\|Si}$-$Ga_2O_{3\|Ga1}$	0.45	0.11	2.43	Type-II
$SiC_{\|Si}$-$Ga_2O_{3\|OGa2}$	0.06	0.27	3.35	Type-I
$SiC_{\|Si}$-$Ga_2O_{3\|OGa1}$	0.02	0.42	3.22	Type-I
$SiC_{\|C}$-$Ga_2O_{3\|Ga2}$	0.61	0.09	2.75	Type-II
$SiC_{\|C}$-$Ga_2O_{3\|Ga1}$	0.39	0.23	2.68	Type-II
$SiC_{\|C}$-$Ga_2O_{3\|OGa2}$	0.12	0.29	3.05	Type-I
$SiC_{\|C}$-$Ga_2O_{3\|OGa1}$	0.08	0.42	2.98	Type-I