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

Supplementary Information

Interfacial thermal transport of graphene/β-Ga_2O_3 heterojunction: a molecular dynamics study with a self-consistent interatomic potential

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1. Lattice parameters of β-Ga_2O_3

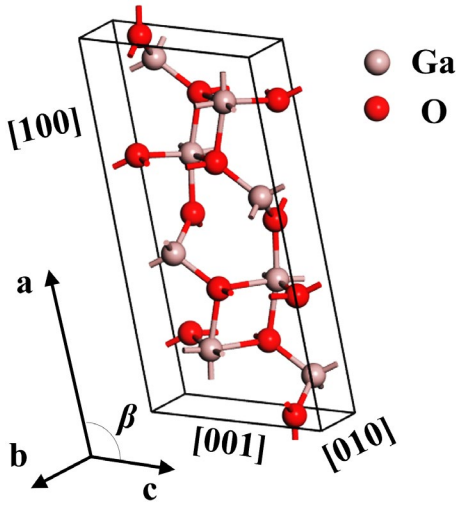

Figure S1. The conventional unit cell of the bulk β-Ga_2O_3.

Table S1. The optimized lattice parameters of β-Ga_2O_3 conventional unit cell.

a	***b***	***c***	***α***	***β***	***γ***	Space group
12.105 Å	3.041 Å	5.897 Å	90°	104.415°	90°	C2/m

2. Fractional coordinates of Ga and O atoms in β-Ga_2O_3

Table S2. The optimized fractional coordinates of Ga and O atoms in the β-Ga_2O_3 lattice structure using GULP.

Atom and number	*x*	*y*	*z*
Ga1	0.0904	0	0.7948
Ga2	0.341036	0	0.684186
O1	0.159875	0	0.106129
O2	0.49356	0	0.253661
O3	0.827145	0	0.431439
Ga3	0.5904	0.5	0.7948
Ga4	0.841036	0.5	0.684186
O4	0.659875	0.5	0.106129
O5	0.99356	0.5	0.253661
O6	0.327145	0.5	0.431439
Ga5	0.908383	0	0.206926
Ga6	0.657747	0	0.31754
O7	0.838908	0	0.895597
O8	0.505223	0	0.748065
O9	0.171638	0	0.570287
Ga7	0.408383	0.5	0.206926
Ga8	0.157747	0.5	0.31754
O10	0.338908	0.5	0.895597
O11	0.005223	0.5	0.748065
O12	0.671638	0.5	0.570287

3. Brillouin zone of monoclinic β-Ga_2O_3 conventional unit cell

Figure S2 depicts the lattice structure, the lattice planes, the Brillouin zone, and the corresponding relationships between the reciprocal lattice vectors and the lattice planes. From Figure S2 (a) we can see that ***a***, ***b*** and ***c*** are along the [100], [010] and [001] crystallographic directions, ***b*** and ***c*** compose the (100) plane, ***a*** and ***c*** compose the (010) plane, ***a*** and ***b*** compose the (001) plane. The lattice vectors are given by:

$$\boldsymbol{a}_1^{conv.} = a\vec{x} + 0\vec{y} + 0\vec{z} \tag{S1}$$

$$\boldsymbol{a}_2^{conv.} = 0\vec{x} + b\vec{y} + 0\vec{z} \tag{S2}$$

$$\boldsymbol{a}_3^{conv.} = c \cdot \cos\beta\vec{x} + 0\vec{y} + c \cdot \sin\beta\vec{z} \tag{S3}$$

Based on equations S1-S3, the Brillouin zone of the β-Ga_2O_3 conventional unit cell can be created (see Figure S2 (b)), and $\boldsymbol{g}_1$, $\boldsymbol{g}_2$ and $\boldsymbol{g}_3$ are the reciprocal lattice vectors (see Figure S2 (c)-(e)). The coordinates of high-symmetry points X, Y and Z in Figure S2 (b)-(e) are (0.5, 0, 0), (0, 0.5, 0) and (0, 0, 0.5). From Figure S2 (c)-(e), the high-symmetry points path Γ-X (which is along the reciprocal lattice vector $\boldsymbol{g}_1$) is perpendicular to the (100) plane, the Γ-Y (which is along the reciprocal lattice vector $\boldsymbol{g}_2$) is perpendicular to the (010) plane, and the Γ-Z (which is along the reciprocal lattice vector $\boldsymbol{g}_3$) is perpendicular to the (001) plane in real space.

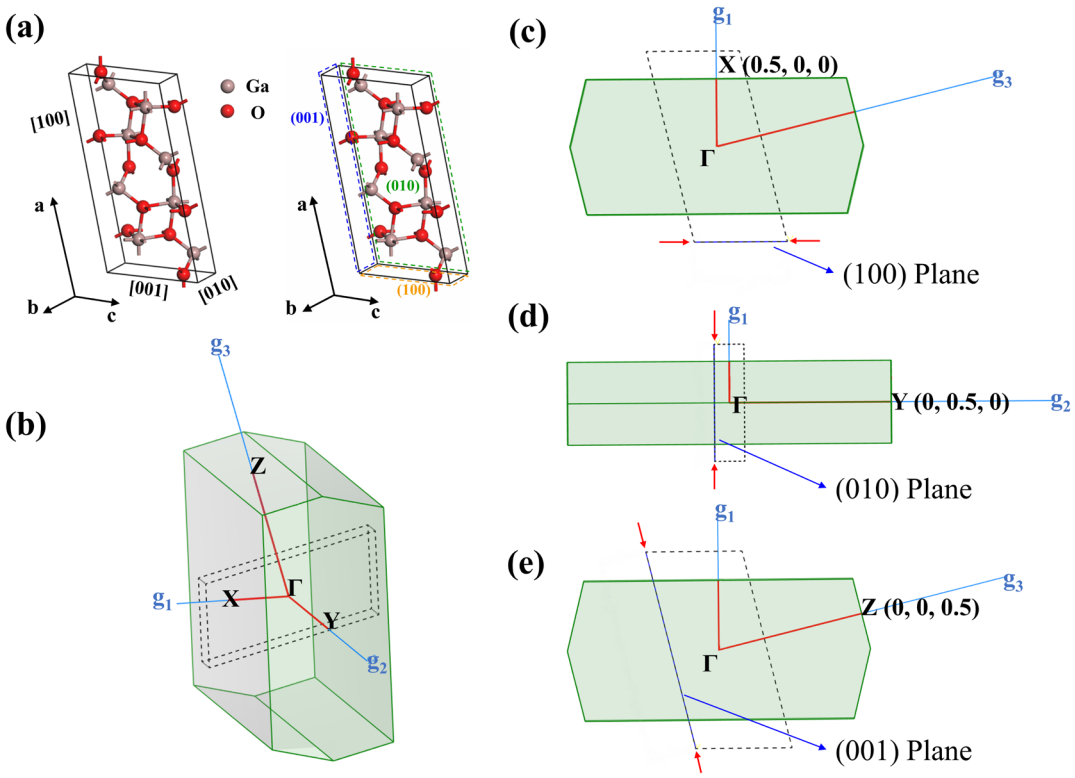

Figure S2. (a) The lattice structure and three typical planes of monoclinic β-Ga_2O_3 conventional unit cell. (b) The Brillouin zone of monoclinic β-Ga_2O_3 conventional unit cell. (c)-(e) The indications of (100), (010) and (001) lattice planes. The three reciprocal lattice vectors are indicated using $\boldsymbol{g_1}$, $\boldsymbol{g_2}$ and $\boldsymbol{g_3}$. Γ (0,0,0), X (0.5,0,0), Y (0,0.5,0) and Z (0,0,0.5) are high-symmetry points of the Brillouin zone.