Supplementary materials

Controlled polarity-inversion in GaAs/Ge/GaAs{111} heterostructures

Akihiro Ohtake[*,†] *and Yusuke Hayashi*[†]

[†]*National Institute for Materials Science (NIMS), Tsukuba 305-0044, Japan*
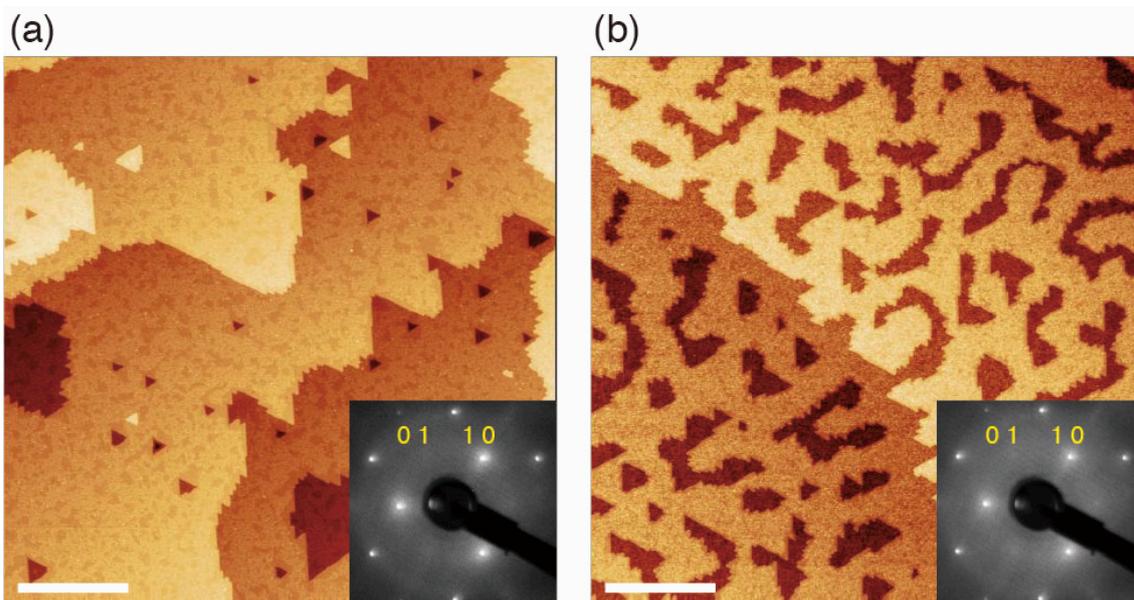
Corresponding Author: OHTAKE.Akihiro@nims.go.jp

Figure S1. STM images of 10 BL-Ge films grown on the GaAs(111)A-(2x2) (a) and (111)B-($\sqrt{19}$x$\sqrt{19}$) (b) substrates. The images were taken with a bias voltage of -3.0 V. Image dimensions are 500 nm x 500 nm (scale bars: 100 nm). The insets show corresponding LEED patterns (182 eV).

Figure S2. RHEED patterns (A-F) and STM images (G-I) taken during the growth of GaAs(111)A/Ge/GaAs(111)A (a) and GaAs(111)B/Ge/GaAs(111)A (b) heterostructures on the (111)A-oriented substrates. RHEED patterns were taken along the [-101] azimuth of the GaAs(111)A substrate; (A) initial GaAs substrate, (B) 10 BL-Ge film, (C) Ga- (a) and In- (b) terminated Ge films, (D) 10 BL-GaAs films (as-grown) (E) 10 BL-GaAs films (after annealing), and (F) 30 BL-GaAs films (after annealing). STM images in (G), (H), and (I) were taken from the 10 BL-GaAs film (as-grown), 10BL-GaAs film (after annealing), and 30 BL-GaAs film, respectively, with a bias voltage of −3V. Image dimensions are 500 nm x 500 nm. (J) shows a schematic drawing of the heterostructure.
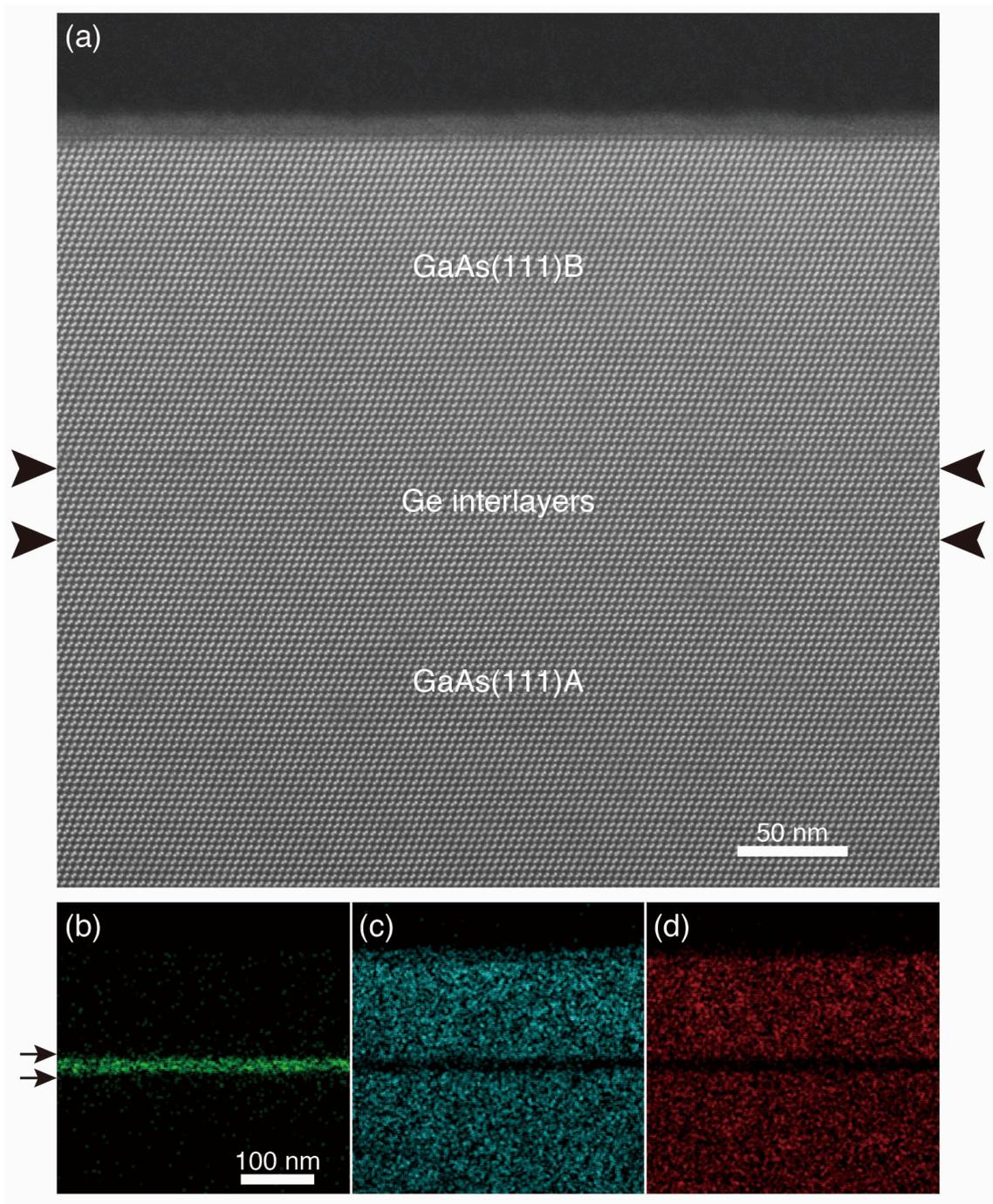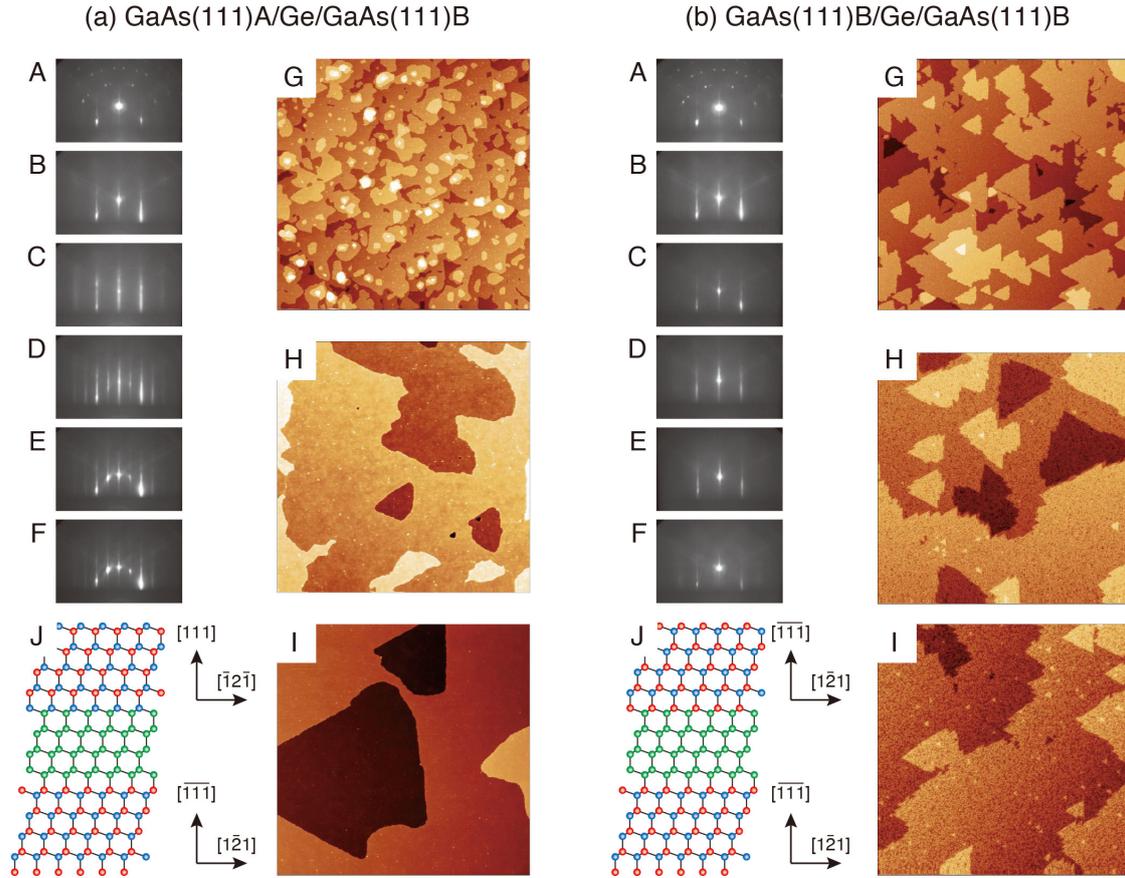
Figure S3. (a) High-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM) image of the GaAs(111)B/Ge (10 BL)/GaAs(111)A structure. (b)-(d) show energy dispersive x-ray spectroscopy (EDX) images with the Ge-K (green), Ga-K (blue), and As-K (red) lines, respectively. Allows indicate the position of interfaces.

(a) GaAs(111)A/Ge/GaAs(111)B

(b) GaAs(111)B/Ge/GaAs(111)B

A

B

C

D

E

F

G

H

I

J

[111]

[ī2ī]

[ī1̄1̄]

[1̄21]

A

B

C

D

E

F

G

H

I

J

[ī1̄1̄]

[1̄2̄1]

[ī1̄1̄]

[1̄2̄1]

Figure S4. RHEED patterns (A-F) and STM images (G-I) taken during the growth of GaAs(111)A/Ge/GaAs(111)A (a) and GaAs(111)B/Ge/GaAs(111)A (b) heterostructures on the (111)A-oriented substrates. RHEED patterns were taken along the [10-1] azimuth of the GaAs(111)B substrate; (A) initial GaAs substrate, (B) 10 BL-Ge film, (C) Ga- (a) and In- (b) terminated Ge films, (D) 10 BL-GaAs films (as-grown) (E) 10 BL-GaAs films (after annealing), and (F) 30 BL-GaAs films (after annealing). STM images in (G), (H), and (I) were taken from the 10 BL-GaAs film (as-grown), 10BL-GaAs film (after annealing), and 30 BL-GaAs film, respectively, with a bias voltage of −3V. Image dimensions are 500 nm x 500 nm. (J) shows a schematic drawing of the heterostructure.
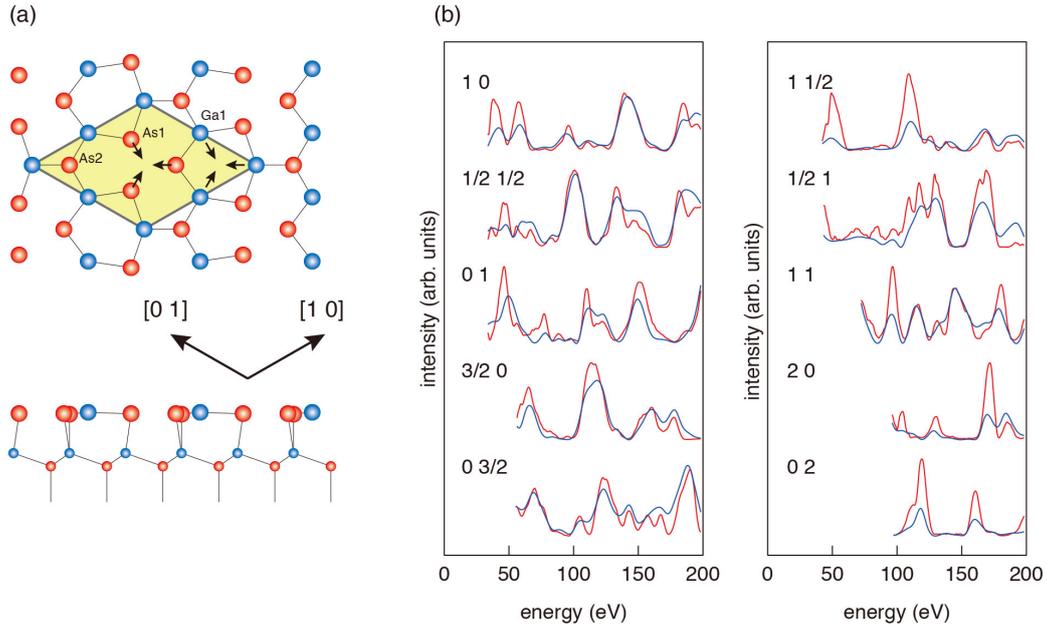
Figure S5. (a) Structure model for GaAs(111)A-(2x2). (b) Measured (red) and calculated (blue) LEED I−V curves. LEED I−V curves were calculated using SATLEED package provided by Barbieri and Van Hove [1,2]. The Ga vacancy-buckling structure (a) yields the Pendry's reliability factor [3] of 0.29, showing a good agreement with the LEED experiments. The structure parameters in the optimized model (Fig. S5(a)) are listed in Table S1.

Table S1. Atomic displacements from bulk positions in the vacancy buckling structure for GaAs(111)A-(2x2) in Å. The (+) and (−) values denote the upward and downward vertical displacement, respectively, and the directions of lateral displacements are indicated by arrows in Fig. S5(a). The atomic coordinates obtained from the LEED analysis agree well with those reported earlier [4-6].

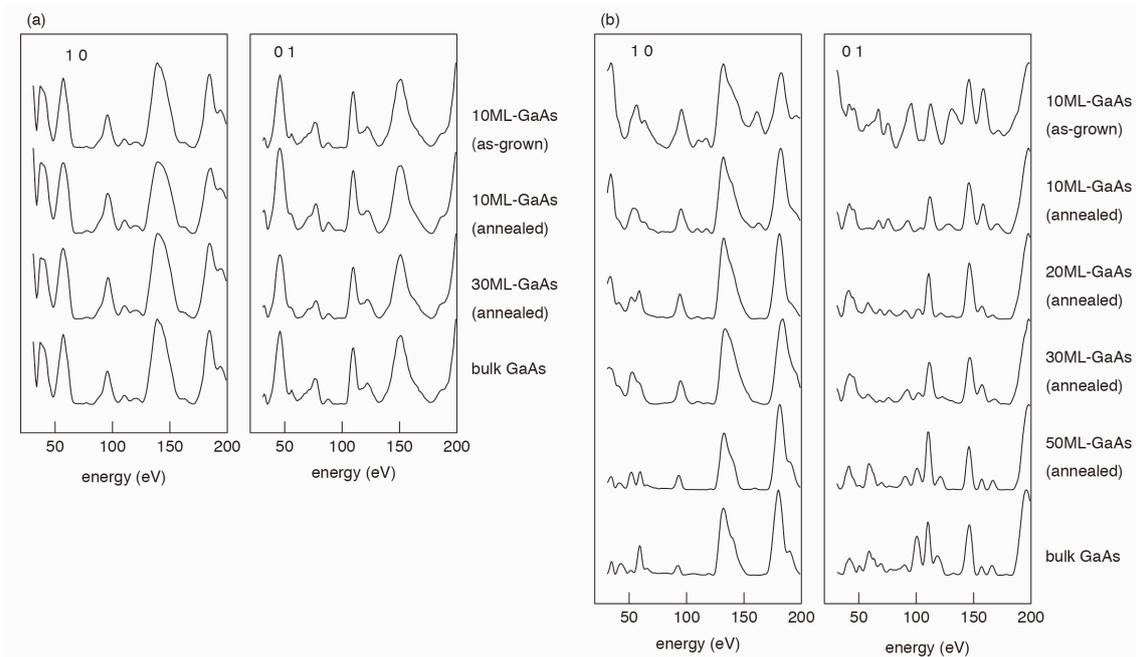|	Ga1		As1		As2	
	lateral	vertical	lateral	vertical	lateral	vertical
This study	0.21	−0.75	0.33	+0.02	---	−0.02
RHEED [4]	0.25	−0.68	0.33	+0.06	---	+0.04
DFT calculations [4]	0.18	−0.61	0.35	+0.20	---	+0.02
LEED [5]	0.1	−0.71	0.28	+0.04	---	−0.08
Tight-binding calculations [6]	0.15	−0.58	0.30	+0.06	---	−0.08

Figure S6. LEED I-V curves measured from GaAs(111)A (a) and GaAs(111)B (b) films. While the I-V curves measured from the GaAs(111)B films change their shapes as the growth proceeds, those measured from the GaAs(111)A films do not show such a change.

References

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