Lattice mismatches of vertical 2D/3D semiconductor heterostructures

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Abstract

Various lattice mismatches at room temperature and 750 °C in van der Waals (vdW) heterostructures of semiconductors were calculated. These calculations propose new substrate for 2D semiconductor synthesis.

It is reported that aligned vertical 2D/3D semiconductor heterostructure is synthesysed in lattice matched system.

In this article, Various lattice mismatch at room temperature and 750 °C in van der Waals (vdW) heterostructures of semiconductor was calculated. The calculation proposes new substrate for 2D semiconductor synthesis. This calculation suggests $MoSe_2$/ZnO is a lattice-matched 2D/3D semiconductor heterostructure with low mismatch.

Keywords: Semiconductor, MoS_2, $MoSe_2$, GaN, ZnO, epitaxy, heterostructure.

I. Introduction

Same planar structures and similar lattice constants are required for epitaxial alignment. Furthermore, these stacks should have similar lattice constants at hot growth temperature, because of these stacks are usually grown in hot growth temperature and cooled down to room temperature.

II. Lattice mismatches at room temperature.

In order to find lattice matched 2D/3D semiconductor systems, lattice parameters of semiconductor materials were surveyed firstly.

formula	polymorph	structure	a	b	c	effective a	Ref
MoS_2		hexagonal	3.162		12.29		[1]
$MoSe_2$		hexagonal	3.288		12.93		[1]
$MoTe_2$		hexagonal	3.519		13.964		[2]
C	Graphene	hexagonal	0.246		N/A		[3]
C	Graphite	hexagonal	0.2461		6.708		[4]
C	Diamond	FCC diamond-cubic	3.567			2.522	[5]
Si	Silicon	FCC diamond-cubic	5.431			3.84	[6]
SiC	(β)3C-SiC	zincblende	4.3596			3.0827	[7]
SiC	4H-SiC	hexagonal	3.073		10.053		[8]
SiC	6H-SiC	hexagonal	3.081		15.12		[9]
Ge		FCC diamond-cubic	5.658			4.001	[6]
BN	c-BN	zincblende	3.615			2.5562	[10]
BN	h-BN	P6m2	2.502		6.66		[11]
BP		zincblende	4.5383			3.2091	[12]
AlN		wurtzite	3.112		4.982		[13]
AlP		zincblende	5.4635			3.8633	[14]
GaN		wurtzite	3.186		5.186		[13]
GaP		zincblende	5.4505			3.8541	[14]
InN		wurtzite	3.533		5.693		[15]
ZnO		wurtzite	3.25		5.2		[16]

Table 1 : Lattice parameters(Å) of Semiconductor materials at room temperature. *effective a* means $\frac{a}{\sqrt{2}}$ for FCC or zincblend structures.

In this table, effective a is $\frac{a}{\sqrt{2}}$, because of (111) plane of FCC structure or (111) plane of Zincblende structure are consist of hexagonal lattice.
Removing unmatched system, the table can be shortened.

formula	polymorph	structure	a	b	c	effective a	Ref
MoS_2		hexagonal	3.162		12.29		[1]
$MoSe_2$		hexagonal	3.288		12.93		[1]
$MoTe_2$		hexagonal	3.519		13.964		[2]
SiC	(β)3C-SiC	zincblende	4.3596			3.0827	[7]
SiC	4H-SiC	hexagonal	3.073		10.053		[8]
SiC	6H-SiC	hexagonal	3.081		15.12		[9]
BP		zincblende	4.5383			3.2091	[12]
AlN		wurtzite	3.112		4.982		[13]
GaN		wurtzite	3.186		5.186		[13]
InN		wurtzite	3.533		5.693		[15]
ZnO		wurtzite	3.25		5.20		[16]

Table 2 : Lattice parameters(Å) of Semiconductor materials at room temperature. *effective a* means $\frac{a}{\sqrt{2}}$ for FCC or zincblend structures.

This table shows MoS_2/GaN, $MoSe_2$/GaN, $MoSe_2$/ZnO, MoS_2/SiC, MoS_2/AlN, $MoTe_2$/InN and MoS_2/BP are lattice matched semiconductor systems. Lattice mismatches are

calculated by this formula; $\frac{a_{substrate} - a_{2D\,layer}}{a_{substrate}}$.

heterostructure	substrate structure	*effective* a(Å) (substrate)	a(2D layer) (Å)	mismatch(%)	Ref
MoS_2/(β)3C-SiC	zincblende	3.0827	3.162	-2.57%	[1][7]
MoS_2/4H-SiC	hexagonal	3.073	3.162	-2.90%	[1][8]
MoS_2/6H-SiC	hexagonal	3.081	3.162	-2.63%	[1][9]
MoS_2/BP	zincblende	3.2091	3.162	3.12%	[1][12]
MoS_2/AlN	wurtzite	3.112	3.162	-1.61%	[1][13]
MoS_2/GaN	wurtzite	3.186	3.162	0.76%	[1][13]
$MoSe_2$/GaN	wurtzite	3.186	3.288	-3.20%	[1][13]
$MoTe_2$/InN	wurtzite	3.533	3.519	0.396%	[2][15]
$MoSe_2$/ZnO	wurtzite	3.25	3.288	-1.17%	[1][16]

Table 3 : Lattice mismatch of Semiconductor heterostructure at room temperature. *effective a* means $\frac{a}{\sqrt{2}}$ for FCC or zincblend structures. Negative sign means 2D layer is compressed.(Lattice of 2D layer is bigger than that of substrate)

Every in-plane lattice mismatches in Table 2 are not bigger than 3.20%.

III. Lattice constants of 2D layers at 750 °C

III.1. MoS_2

Lattice constants of MoS_2 in the range 20 to 850 °C were given as second-order polynomials by S. H. El-Mahalawy and B. L. Evans. [17]

$a = 3.1621 + 0.6007 \times 10^{-5}t + 0.3479 \times 10^{-7}t^2$
$c = 12.3024 + 0.1064 \times 10^{-3}t + 0.7737 \times 10^{-7}t^2$

In 750 °C, *a* = 3.1862 Å, *c* = 12.426 Å by this formula.

III.2. $MoSe_2$

Lattice constants of $MoSe_2$ in the range 20 to 850 °C were given as second-order polynomials by S. H. El-Mahalawy and B. L. Evans. [17]
$a = 3.2910 + 0.2382 \times 10^{-4}t + 0.0118 \times 10^{-7}t^2$
$c = 12.9288 + 0.1672 \times 10^{-3}t - 0.4987 \times 10^{-7}t^2$ (unit: Å, t: °C)

In 750 °C, *a* = 3.3095 Å, *c* = 13.026 Å by this formula.

IV. Lattice constants of 3D semiconductor substrates at 750 °C

IV.1. GaN

Graph of Lattice constants of GaN was given by Maruska and H.P, Tietjen.[18]

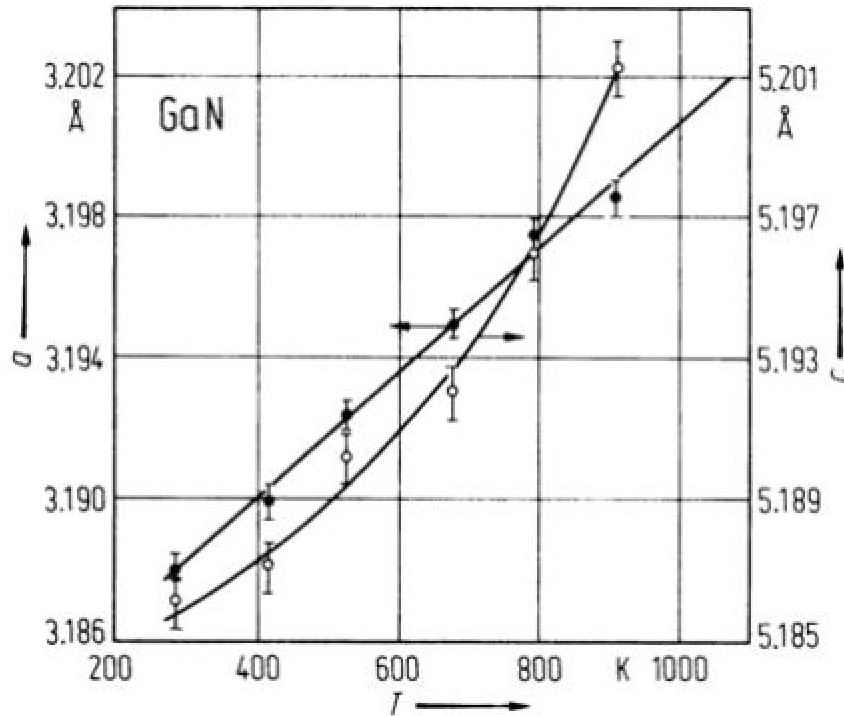

Figure 1 Lattice constants of GaN.[18]
Lattice constant of GaN at 750 °C can be achieved by interpolation: a = 3.196 Å, c = 5.194 Å .

IV.2. ZnO

Aijaz A.Khan determined lattice parameters of zinc oxide.[18]
Thermal expansion coefficients of zinc oxide were given by this result;

$\alpha_a = 6.05\times10^{-6} + 2.20\times10^{-9}t + 2.29\times10^{-12}t^2$
$\alpha_c = 3.53\times10^{-6} + 2.38\times10^{-9}t + 9.24\times10^{-14}t^2$ (t :°C, α: °C^{-1})

Then,
$\int\alpha_a = 6.05\times10^{-6}t + 2.20\times10^{-9}t^2/2 + 2.29\times10^{-12}t^3/3$
$\int\alpha_c = 3.53\times10^{-6}t + 2.38\times10^{-9}t^2/2 + 9.24\times10^{-14}t^3/3$
Lattice constant of ZnO at 750 °C are
$a_{750\ °C} = a_{619°C}\ e^{\int\alpha_a}$ = 3.2674 Å, $c_{750\ °C} = c_{619°C}\ e^{\int\alpha_c}$ =5.2240 Å.

IV.3. SiC

IV.3.1. 3H-SiC

3C-SiC has zincblende structure. (111) plane of 3C-SiC is consisted of hexagonal lattice. Lattice constant of 3H-SiC at room temperature was given by Eds. O'Connor *et al.*[19]: a = 4.3596 Å.

This result means effective lattice constant($a_{effective} = \frac{a}{\sqrt{2}}$) at room temperature is 3.0827 Å.
Thermal expansion coefficients of 3H-SiC were given as second-order polynomials by Z. Li and R. C. Bradt.[20]
$\alpha_{(3c)} = 3.19\times10^{-6} + 3.60\times10^{-9}t - 1.68\times10^{-12}t^2$

$\int\alpha_{(3c)} = 3.19\times10^{-6}t + 3.60\times10^{-9}t^2/2 - 1.68\times10^{-12}t^3/3$ (unit: Å, t: °C)

Lattice constants of 3C-SiC at 750 °C are
$a_{750\ °C}=a\ e^{\int\alpha(3c)} = 4.3731$ Å, $a_{750\ °C,effective} = a_{effective}\ e^{\int\alpha(3c)} = 3.0922$ Å

IV.3.2. 4H-SiC

4H-SiC has wurtzite structure. Lattice constants of 4H-SiC at room temperature were given by M. Katz *et al.*[22]: a = 3.073 Å, c = 10.053 Å

Thermal expansion coefficients of 4H-SiC were given as second-order polynomials by Z. Li and R. C. Bradt.[20]
$\alpha_{a(4H)} = 3.21\times10^{-6} + 3.56\times10^{-9}t - 1.62\times10^{-12}t^2$
$\int\alpha_{a(4H)} = 3.21\times10^{-6}t + 3.56\times10^{-9}t^2/2 - 1.62\times10^{-12}t^3/3$
$\alpha_{c(4H)} = 3.09\times10^{-6} + 2.63\times10^{-9}t - 1.08\times10^{-12}t^2$
$\int\alpha_{c(4H)} = 3.09\times10^{-6}t + 2.63\times10^{-9}t^2/2 - 1.08\times10^{-12}t^3/3$ (unit: Å, t: °C)

Lattice constants of 4H-SiC at 750 °C are
$a_{750\ °C}=a\ e^{\int\alpha_a(4H)} = 3.0825$ Å, $c_{750\ °C}=c\ e^{\int\alpha_c(4H)} = 10.082$ Å

IV.3.3. 6H-SiC

6H-SiC has wurtzite structure. Lattice constants of 6H-SiC at room temperature were given by D. G. Zhao *et al.*[22]: a = 3.081 Å, c = 15.12 Å

Thermal expansion coefficients of 6H-SiC were given as second-order polynomials by Z. Li and R. C. Bradt.[20]

$\alpha_{a(6H)} = 3.27\times10^{-6} + 3.25\times10^{-9}t - 1.36\times10^{-12}t^2$
$\int\alpha_{a(6H)} = 3.27\times10^{-6}t + 3.25\times10^{-9}t^2/2 - 1.36\times10^{-12}t^3/3$
$\alpha_{c(6H)} = 3.18\times10^{-6} + 2.48\times10^{-9}t - 8.51\times10^{-13}t^2$
$\int\alpha_{c(6H)} = 3.18\times10^{-6}t + 2.48\times10^{-9}t^2/2 - 8.51\times10^{-13}t^3/3$ (unit: Å, t: °C)

Lattice constants of 3C-SiC at 750 °C are
$a_{750\ °C}=a\ e^{\int\alpha_a(6H)} = 3.0905$ Å, $c_{750\ °C}=c\ e^{\int\alpha_c(6H)} = 15.164$ Å.

IV.4. AlN

Lattice constants of AlN were given as second-order polynomials by H. Iwanaga *et al.*[23]

$a = 3.1071 + 1.211 \times 10^{-5}t + 2.36 \times 10^{-9}t^2$
$c = 4.9739 + 1.455 \times 10^{-5}t + 4.65 \times 10^{-9}t^2$ (unit: Å, t: K)

Lattice constants of 3C-SiC at 750 °C can be calculated by these polynomials; a = 3.1220 Å, c = 4.9937 Å.
V. Lattice parameters and lattice mismatches at 750 °C.

formula	polymorph	structure	a	b	c	effective a
MoS_2		hexagonal	3.1862		12.426	
$MoSe_2$		hexagonal	3.3095		13.026	
SiC	(β)3C-SiC	zincblende	4.3731			3.0922
SiC	4H-SiC	hexagonal	3.0825		10.082	
SiC	6H-SiC	hexagonal	3.0905		15.164	
AlN		wurtzite	3.1220		4.9937	
GaN		wurtzite	3.196		5.194	
ZnO		wurtzite	3.2674		5.2240	

Table 4 : Lattice parameters(Å) of Semiconductor materials at 750 °C. *effective a* means $\frac{a}{\sqrt{2}}$ for FCC or zincblend structures.

heterostructure	substrate structure	*effective* a(Å) (substrate)	a(2D layer) (Å)	mismatch(%)
MoS_2/(β)3C-SiC	zincblende	3.0922	3.1862	-3.04%
MoS_2/4H-SiC	hexagonal	3.0825	3.1862	-3.36%
MoS_2/6H-SiC	hexagonal	3.0905	3.1862	-3.10%
MoS_2/AlN	wurtzite	3.1220	3.1862	-2.06%
MoS_2/GaN	wurtzite	3.196	3.1862	0.31%
$MoSe_2$/GaN	wurtzite	3.196	3.3095	-4.096%
$MoSe_2$/ZnO	wurtzite	3.2674	3.3095	-1.29%

Table 5 : Lattice mismatch of Semiconductor heterostructure at 750 °C. *effective a* means $\frac{a}{\sqrt{2}}$ for FCC or zincblend structures. Negative sign means 2D layer is compressed.(Lattice of 2D layer is bigger than that of substrate)

VI. Conclusion

Epitaxial aligned heterostructure of $MoSe_2$ and ZnO is expected because in-plane lattice mismatch of $MoSe_2$ and ZnO are less than 1.3% for room temperature and growth temperature. Furthermore, It is expected that ZnO could facilitate $MoSe_2$ deposition to form $MoSe_2$/ZnO heterostructure. Cation-polar substrate of Wurtzite structure promotes the absorption of anions because the substrate is uniformly terminated with cation.[24]

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