SiC/SiO_2の特性と膜生成法

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2021/7/15(Thu)押山先生PJ MTG

Background: Why SiC?

・SiC application is already started as a power-device semiconductor.
・SiC-power devices start to replace Si-power devices in many places.

エアコン (三菱、ダイキン 2010~)
太陽電池用パワコン、サーバー電源

鉄道 (小田急/東京メトロ/JR山手線/環状線など)

MITSUBISHI ELECTRIC
Changes for the Better

N700S
2020年7月~

3300 V - 1500 A SiCモジュール
走行電力 20~36% 低減
変換器体積 80% 低減
http://www.mitsubishielectric.co.jp/news/2014/0430.html

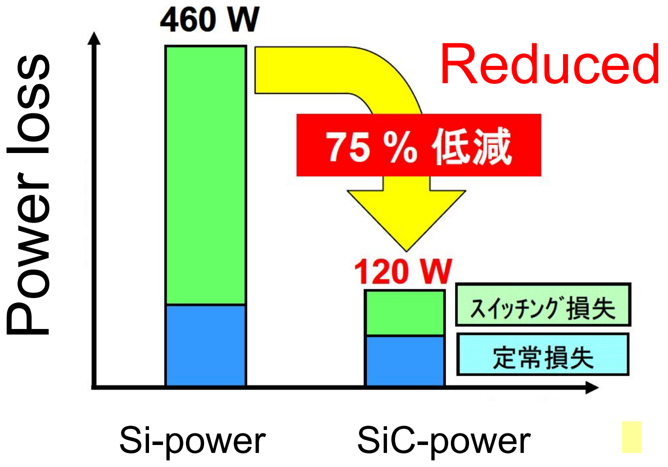
電気自動車 (EV) にSiC
MOSFET + SBD搭載

HONDA FCV
販売 (SiC搭載)

TESLA Model 3 はベストセラー
(月産 2~3 万台)

http://www.honda.co.jp/news/2016/4160310.html
https://www.statista.com/chart/16948/total-number-of-premium-cars-sold-in-the-us/

エレベータ、急速充電器、
高周波加熱用電源 など応用拡大



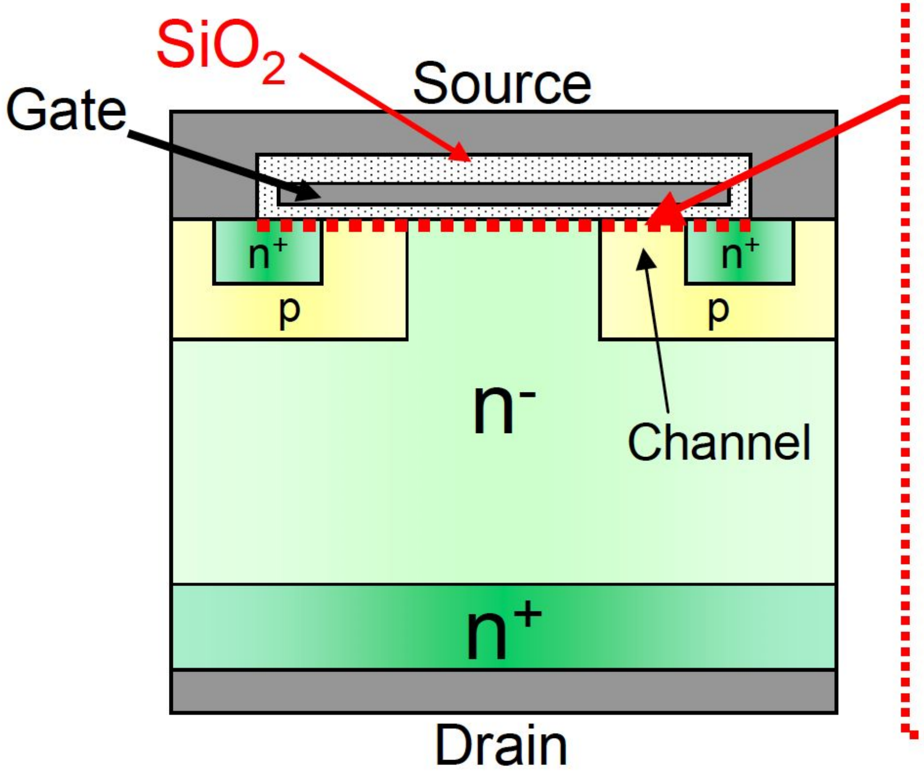
By replacing Si-power devices with SiC, the energy loss can be reduced substantially.

Application of SiC devices is now expanding.

Issue: High density of interface states in SiC-MOS devices

MOS devices are the most important element in power devices.

Cross section of MOSFET



- High density of interfce defects appears at the SiC/SiO_2.

  ~100 times higher than Si/SiO_2

- The interface defects trap electron carriers leading to high resistivity at the interface.

  Electron mobility is only a few percent of theoretical values.
  Actual devices : 20-30 cm2/Vs
  Theoretical value: 1000 cm2/Vs

Reduction of the interface-state density is necessary.

However, identification of the interface states is NOT achieved yet.

Contents

Based on DFT calculations, we have found **an interface-state candidate** and proposed **one process to reduce the interface-state density**.

1, **Interface-state candidate** : Originated from carbon defects

2, **Novel formation process of SiO_2 film** without thermal oxidazation

3, **Summary**

Mystery in the thermal oxidation process of SiC

After the oxidation of SiC, the final products (under enough oxygen and long oxidation time enough) are clear, but...

$$\mathrm{SiC} + 2\mathrm{O}_2 \underline{\underline{\rightarrow ? \rightarrow ?}} \rightarrow \mathrm{SiO}_2 + \mathrm{CO}_2$$

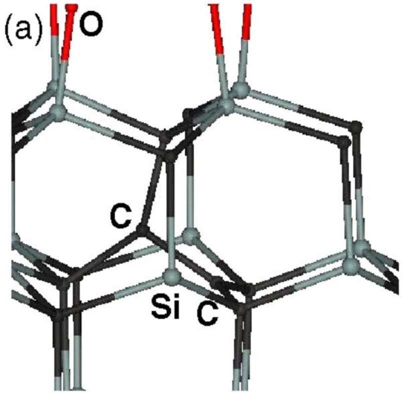
Problem: **Halfway products of carbon species are unclear.**
(Could be related to interface states.
Further, it is not clarified whether the halfway products of carbon species are distributed in the interface area or not.)

Need to identify the halfway products of carbon species

Theoretical preceding works related to carbon defects

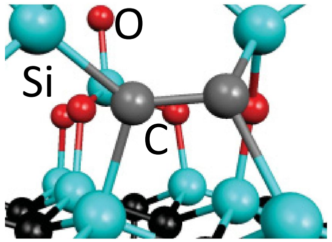
Many DFT calculations performed for carbon related defects.

S. Wang, et al., PRL 98, 026101 (2007).



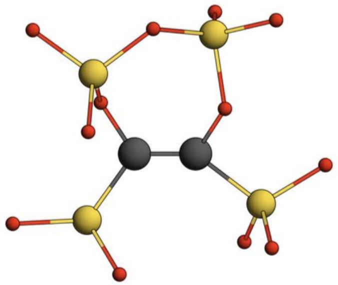
C2 defects distributed in **<u>SiC bulk</u>**

F. Devynck, et al., PRB 83, 195319 (2011).

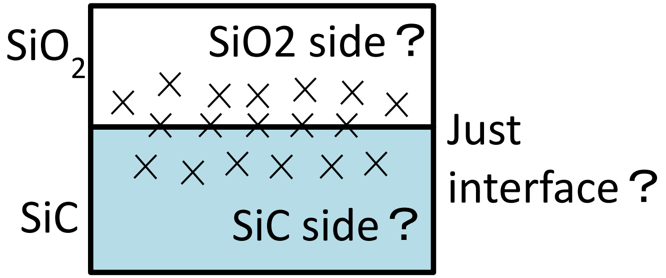


C2 defects distributed at **<u>just the interface</u>**

Knaup, et al., PRB 72, 115323 (2005).



C2 defects distributed in **<u>SiO_2 film</u>**



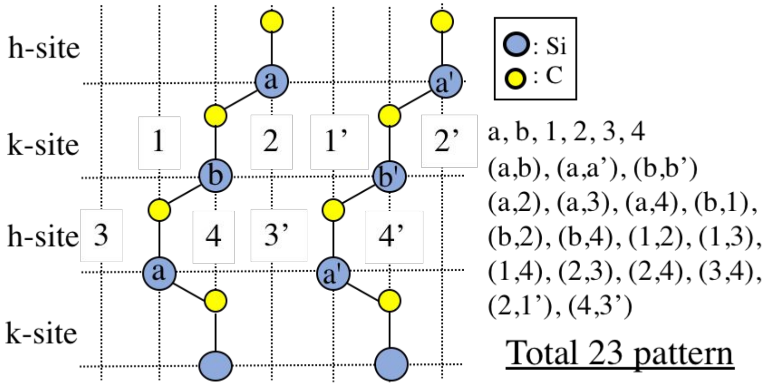
However, still people don't know **which carbon defects are more reasonable one**.

This work

Following the energetics, we have **clarified the stable carbon structures** on the SiC side, SiO2 side, and the just interface on the same footing by comprehensive DFT calculations.

Calculation models (SiC-side・SiO2-side)

SiC-side (All possible C1, C2 defects)

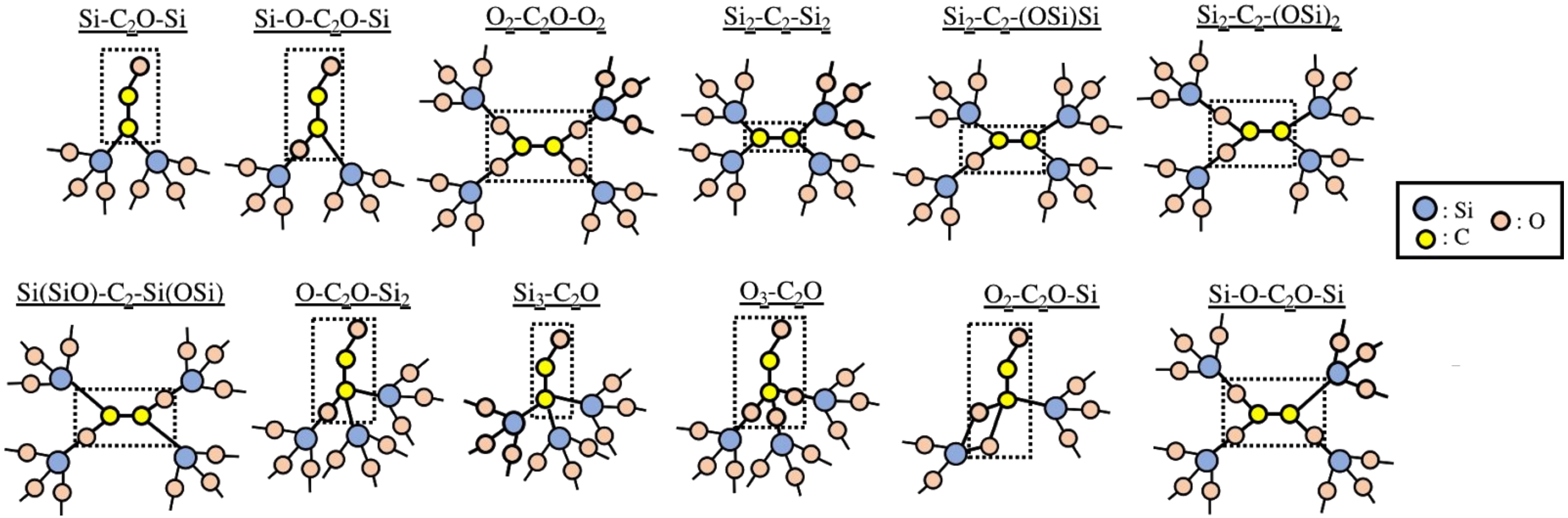


Total 23 defect structures

[1] Y.-I. Matsushita and A. Oshiyama, Jpn. J. Appl. Phys. **57**, 125701 (2018).

SiO2-side (C1, C2 defects screened by CPMD calculations)

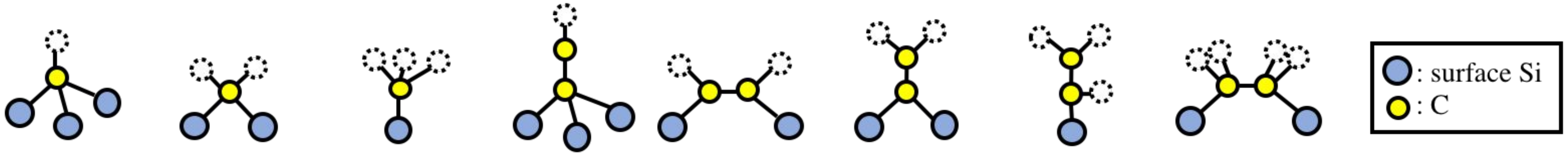
Total 24 defect structures



Calculation models (Just interface)

Just interface (Comprehensive C1, C2 defects)

c1d1 | c1d2 | c1d3 | c2d1 | c2d2h | c2d2v | c2d3 | c2d4



c1d1 — 4 pattern
d, o, h, s

c1d2 — 10 pattern
(d,d), (o,o), (h,h), (s,s), (d,o), (d,h) (d,s), (o,h), (o,s), (s,h)

c1d3 — 20 pattern
(d,d,d), (o,o,o), (h,h,h), (s,s,s), (d,d,o), (d,d,h), (d,d,s), (o,o,d), (o,o,h), (o,o,s), (h,h,d), (h,h,o) (h,h,s),(s,s,d), (s,s,o), (s,s,h), (d,o,h), (d,o,s), (d,h,s), (o,h,s)

c2d1 — 4 pattern
d, o, h, s

c2d2h — 10 pattern
(d,d), (o,o), (h,h), (s,s), (d,o), (d,h) (d,s), (o,h), (o,s), (s,h)

c2d2v — 10 pattern
(d,d), (o,o), (h,h), (s,s), (d,o), (d,h) (d,s), (o,h), (o,s), (s,h)

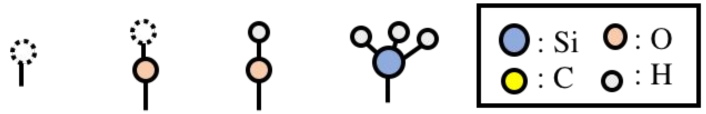
c2d3 — 20 pattern
(d,d,d), (o,o,o), (h,h,h), (s,s,s), (d,d,o), (d,d,h), (d,d,s), (o,o,d), (o,o,h), (o,o,s), (h,h,d), (h,h,o) (h,h,s),(s,s,d), (s,s,o), (s,s,h), (d,o,h), (d,o,s), (d,h,s), (o,h,s)

c2d4 — 1 pattern
(s,s,s,s)

Total:
79 pattern

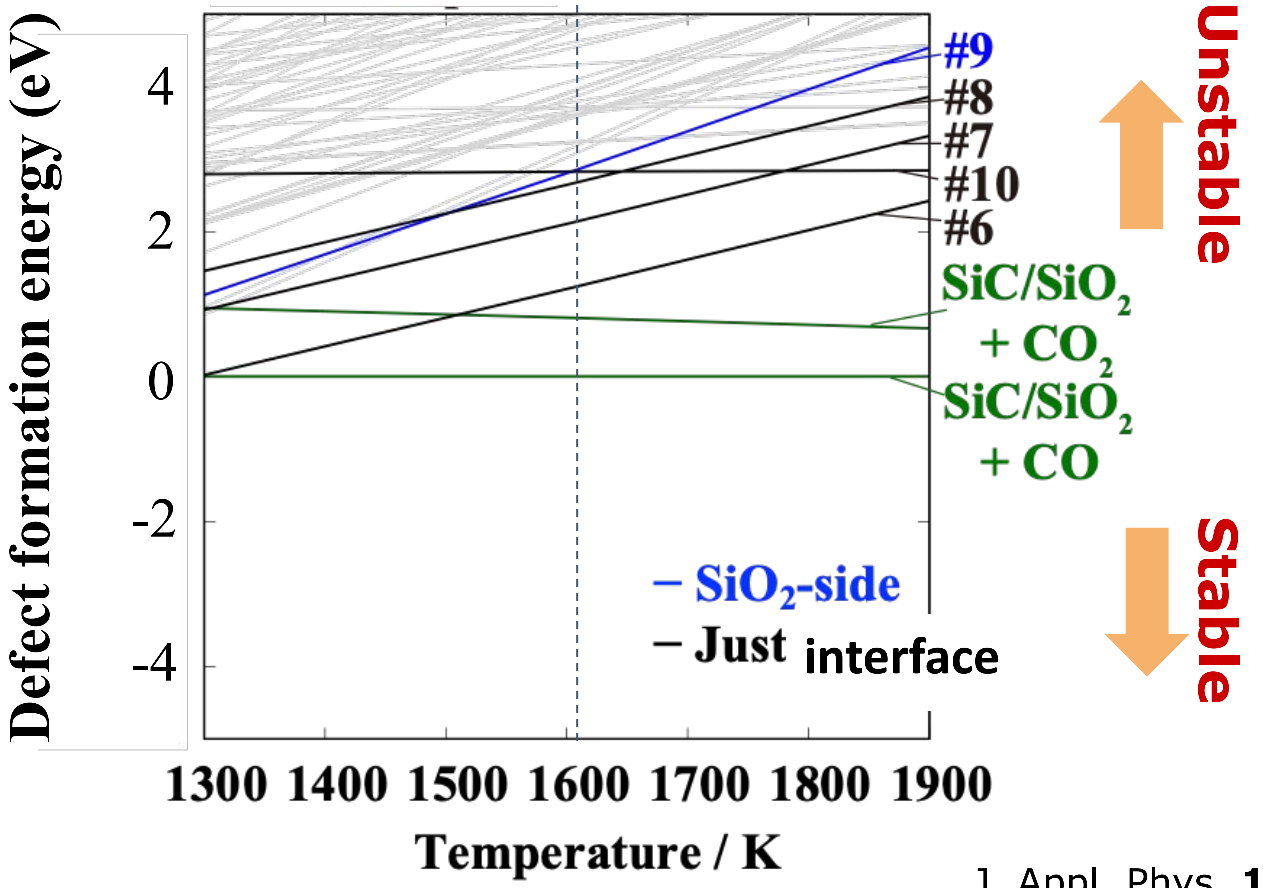
Total 79 defect structures

dangling bond (d) | O (o) | OH (h) | SiH_3 (s)



DFT calculations for the 126 carbon defects

We have performed comprehensive DFT calculations for the 126 carbon defects distributed in the three regions: SiC･SiO2･SiC/SiO2 interfaces.



According to the results:
･Higher oxidation temperature is preferable.
This agrees with experimental fact [1].

[1] T. Hosoi, *et al.*, *Appl. Phys. Lett.* **109**, 182114 (2016).

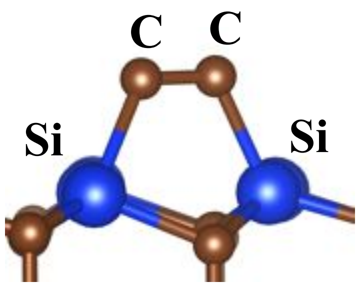
･Carbon defects distributed **at just interface** are stable.

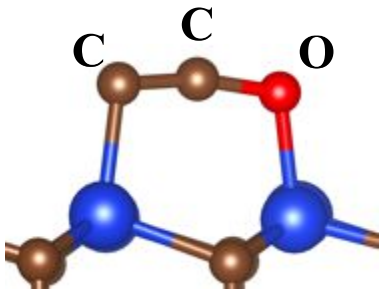
J. Appl. Phys. **126**, 145302 (2019).

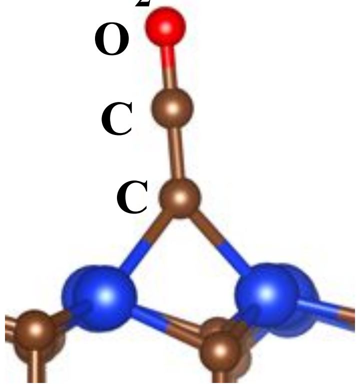
Stable top 5 C-defects at 1600 K

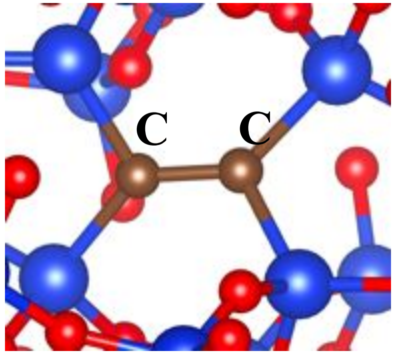
Stable ←

interface	interface	interface	SiO_2-side	interface
#6 Si-C-C-Si	#7 Si-C-C-O-Si	#8 Si_2-C-C-O	#9 Si_2-C-C-Si_2	#10 Si_3-C









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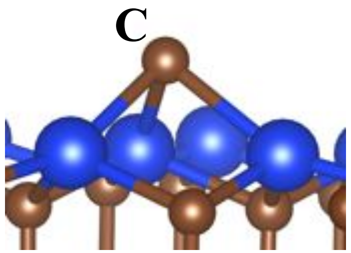


$$\mu_O = (E(SiO_2) - E(Si))/2\ ,\ \mu_{Si} = E\ (Si)\ ,\ \mu_C = E(SiC) - E(Si)$$

- **Of the top five C-defects, four defects are distributed at just interface and only one C-defect on SiO2 side is ranked.**
- **C-dangling bond (#10 Si_3-C) appears as a stable structure**
  : Very recently ESR detected it (Agree with an experimental fact). [1]

[1] Appl. Phys. Lett. **116**, 071604 (2020)

Carbon-related defects likely to be formed and mostly distributed at the interface.

Contents

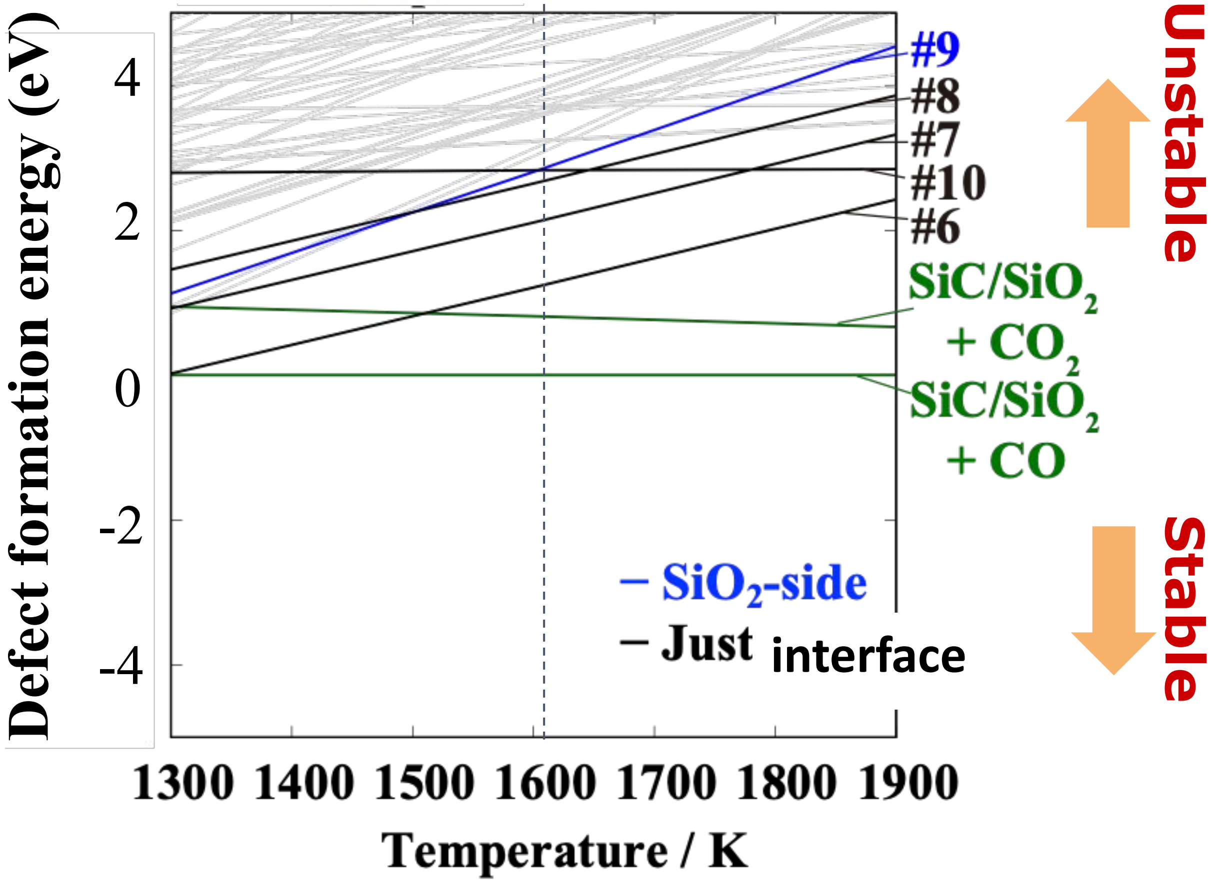
1, **Interface-state candidate** : Originated from carbon defects

Carbon-related defects are formed and mostly distributed at the interface.

2, **Novel formation process of SiO_2 film** without thermal oxidazation

3, **Summary**

More important message from the DFT results



J. Appl. Phys. **126**, 145302 (2019).

Carbon related defects formed in interfaces are energetically stable.

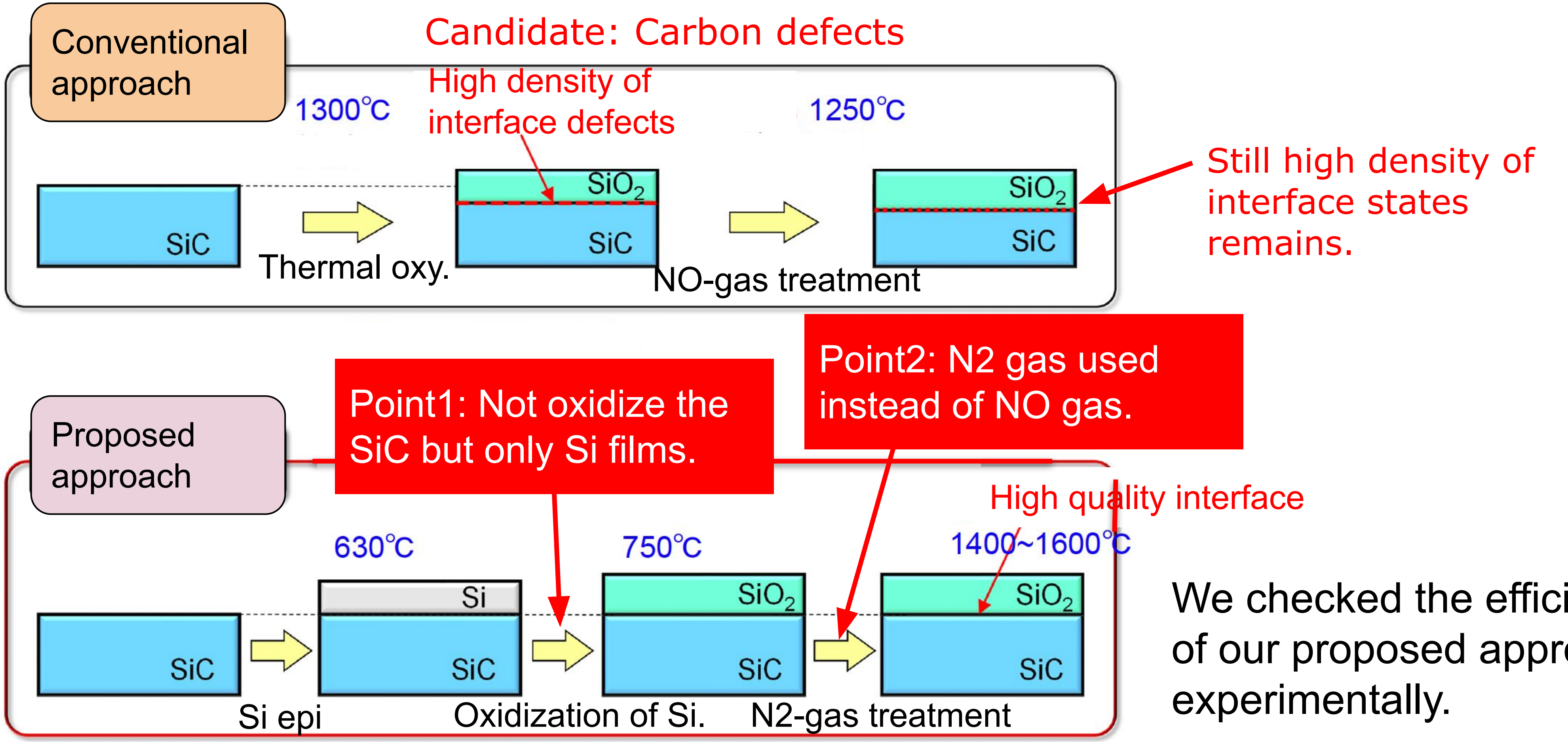
Result1: **As long as thermal oxidation is used**, it means that **carbon defects will inevitably aggregate at the interface.**

Implicit message: If you want to reduce the interface C-defects, **we have to give up the conventional thermal oxidation** to form the SiO2 film.

Novel formation method of SiC/SiO2

Following the DFT results, we proposed a novel formation process of SiO2 film without thermal oxidation.

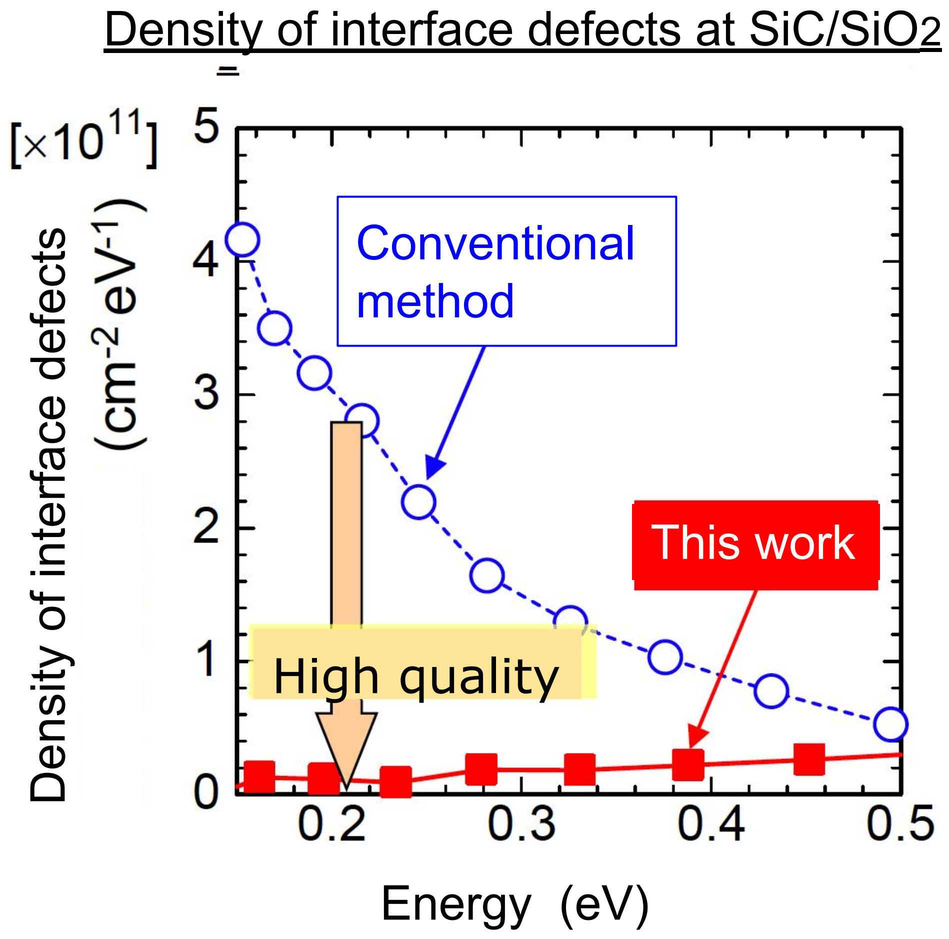
Appl. Phys. Express **13** 091003 (2020).



We checked the efficiency of our proposed approach experimentally.

Great success of our proposed method

Found that **10 times high quality SiC/SiO2 interfaces** realize.



Appl. Phys. Express **13** 091003 (2020).

	Interface-state density
Oxidation only	$1.6x10^{12}$ cm^{-2}
Oxidation+NO treatment	$1.3x10^{11}$ cm^{-2}
This work	$1.2x10^{10}$ cm^{-2}

Density of interface states is reduced substantially **down to 1/10**.

This will make SiC-power devices cheaper down to ~1/10.

Contents

1, **Interface-state candidate** : Originated from carbon defects

Carbon-related defects are formed and mostly distributed at the interface.

2, **Novel formation process of SiO_2 film** without thermal oxidazation

Achieved 10 times higher quality interface reducing the C-defects at the interface

3, **Summary**

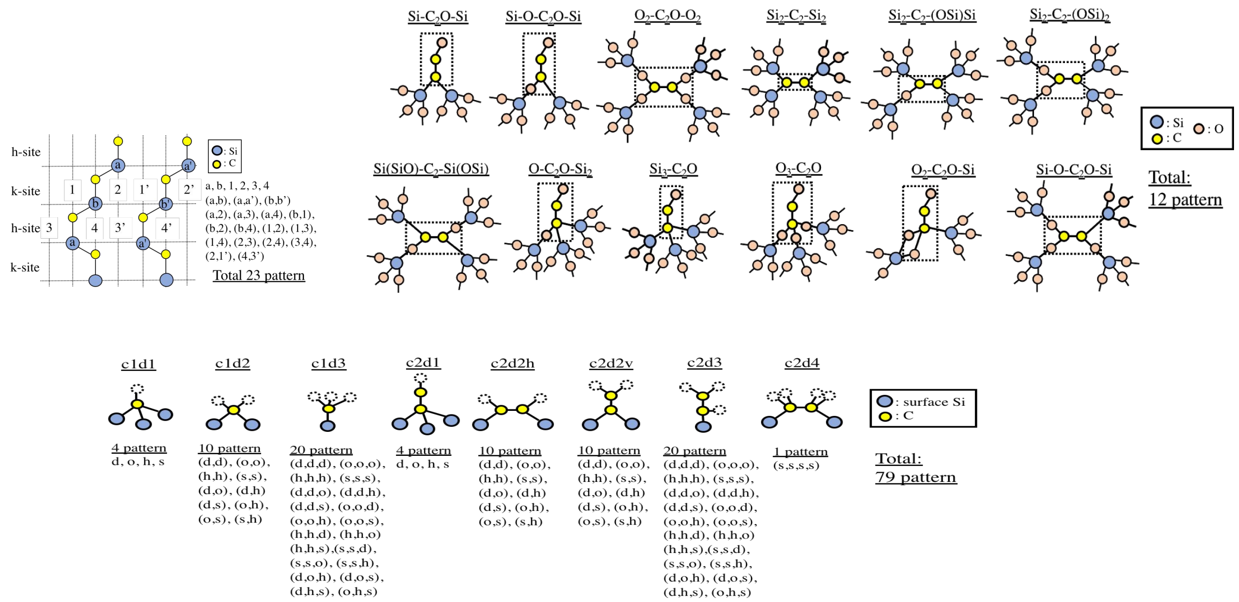
Summary Part 1

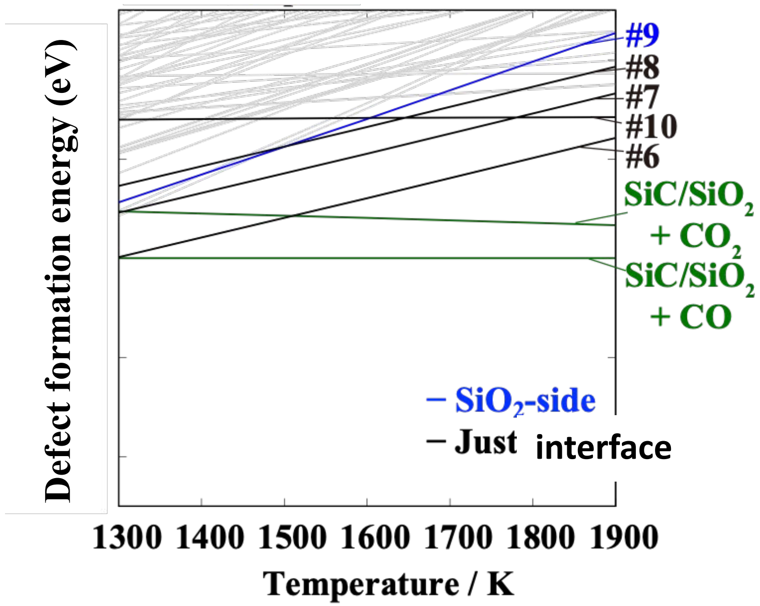
Interface-state candidate : Carbon defects near the SiC/SiO_2

Performed DFT calculations for total 126 carbon defects distributed on SiO2-side, SiC-side, and just interface and clarified the stability among them.

Carbon defects at just interface are energetically favorable.

Found that the thermal oxidation inevitably induces interface defects

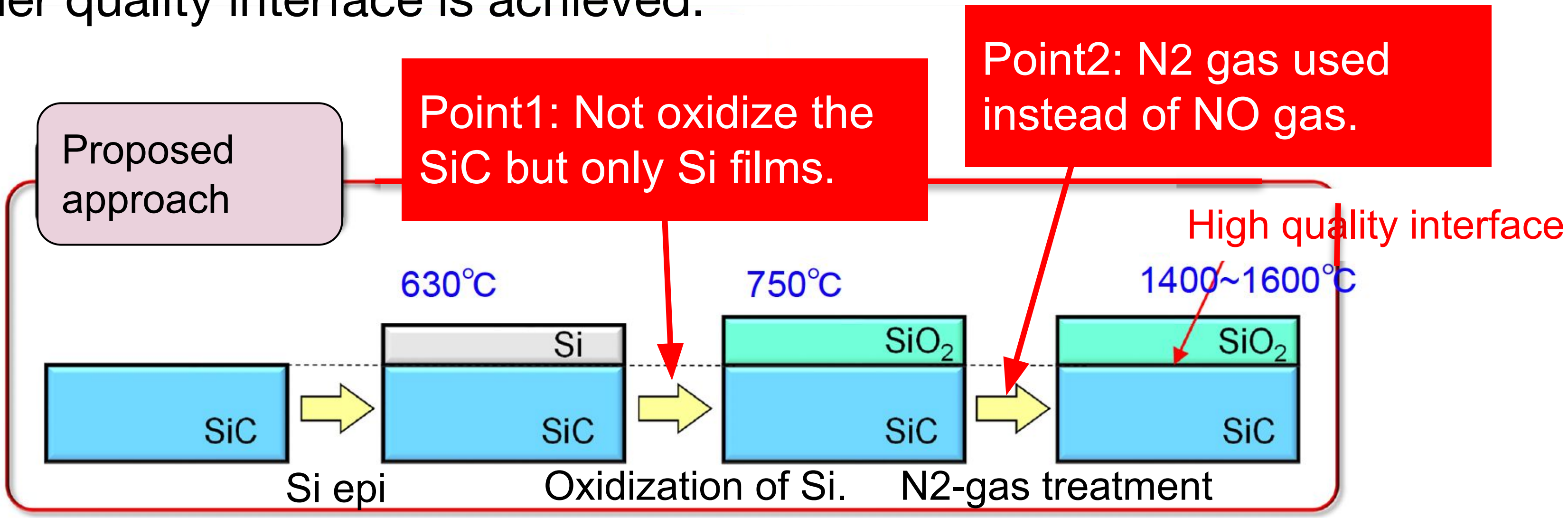


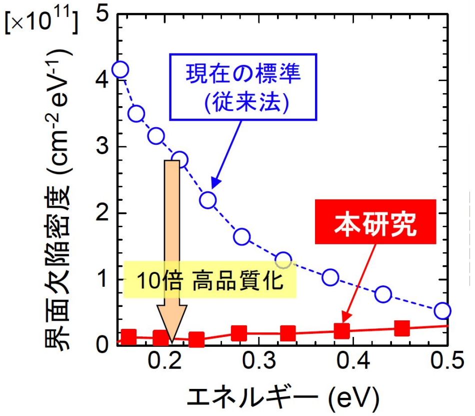


Summary Part 2

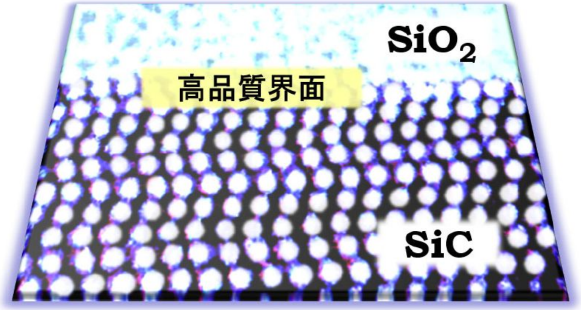
Novel formation process of SiO2 film without thermal oxidazation

10 times higher quality interface is achieved.





Appl. Phys. Express **13** 091003 (2020).



ご清聴ありがとうございました

Thank you for our attention