Manipulation of single spin of NV center in diamond
~ Control of orientation of NV axis ~

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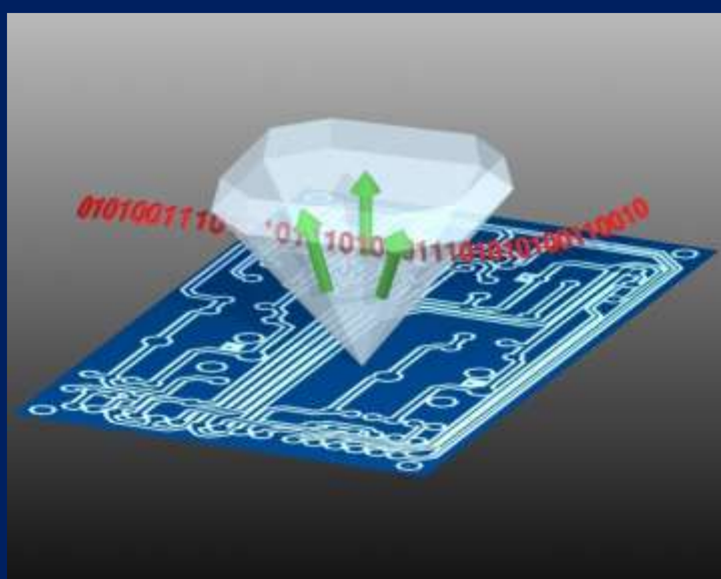

Collaborators and Acknowledgements

- Prof. Suzuki and group members (Osaka Univ.)
- Dr. Yamasaki and group members (AIST)
- Prof. Hatano (Univ. of Tokyo Inst. Tech.), RENESAS
- Dr. Saito, Dr. Matsuzaki, Dr. Munro, Dr. Zhu (NTT)
- Prof. Kosaka (Yokohama Univ.)
- Dr. Semba, (NICT)
- Prof. Nemoto (NII)
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- Prof. F. Jelezko (Ulm Univ.)
- Dr. A. Gali (Wigner Research center.)

Osaka Univ

Content

1. Introduction

   NV center in diamond

2. Selective alignment of N-V axis

   T. Fukui, NM, et al., *Appl. Phys. Exp*. 7, 055201 (2014), selected in "Spotlights"

3. Atomistic mechanism of alignment

   T. Fukui, NM, et al., *Appl. Phys. Exp*. 7, 055201 (2014), selected in "Spotlights"

   T. Miyazaki, NM, et al., *Appl. Phys. Lett*. 105, 261601 (2014).

MATERIALS SCIENCE

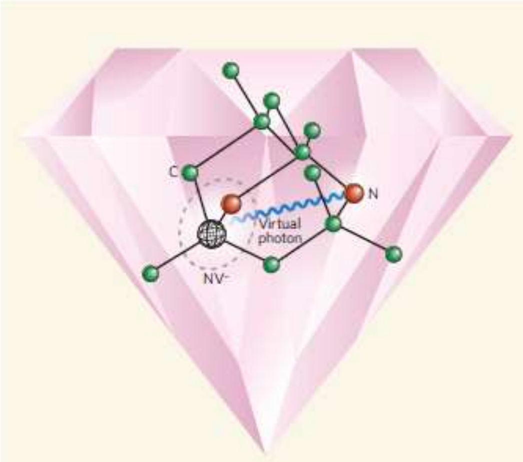
Qubits in the pink

Pieter Kok and Brendon W. Lovett

Crystal imperfections known as nitrogen–vacancy defects give some diamonds a characteristic pink colour. Appropriately manipulated, these defects might have rosy prospects as the 'qubits' of a quantum computer.

According to materials scientist F. C. Franck, "crystals are like people; it is only the defects that make them interesting". Ronald Hanson and colleagues would probably agree: writing in *Physical Review Letters*[1], they report new developments in the study of negatively charged 'nitrogen–vacancy defects' in diamond. These systems are rapidly becoming a front-runner for use as the basic unit of quantum information — the 'qubit' — in a solid-state quantum computer.

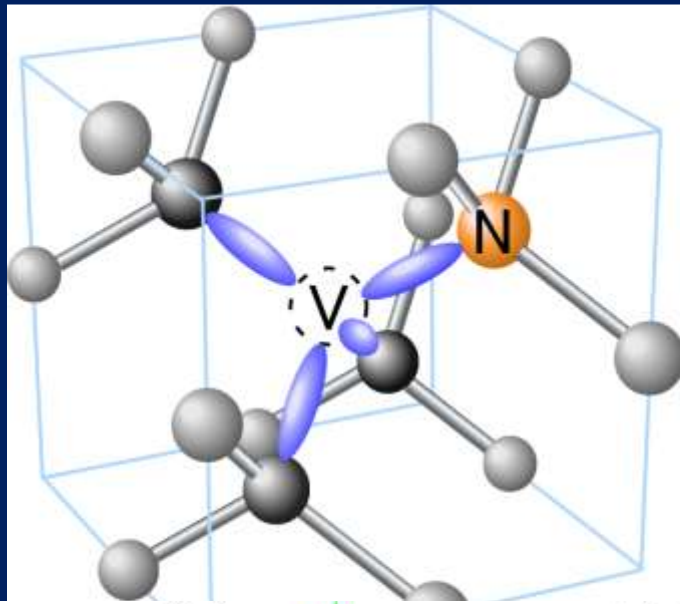
The lattice of carbon atoms that makes up diamond can contain various substitutional impurities, such as nitrogen or boron atoms. These defects give diamonds their colour, and are

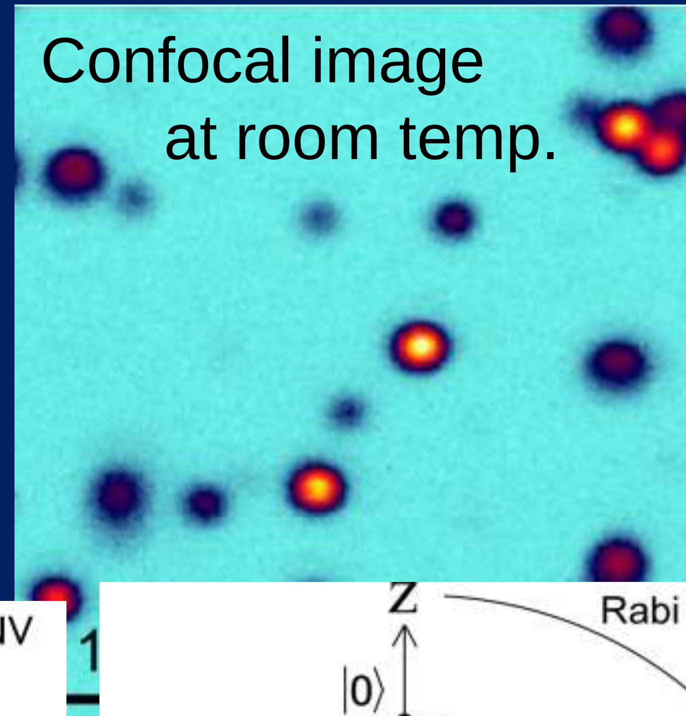


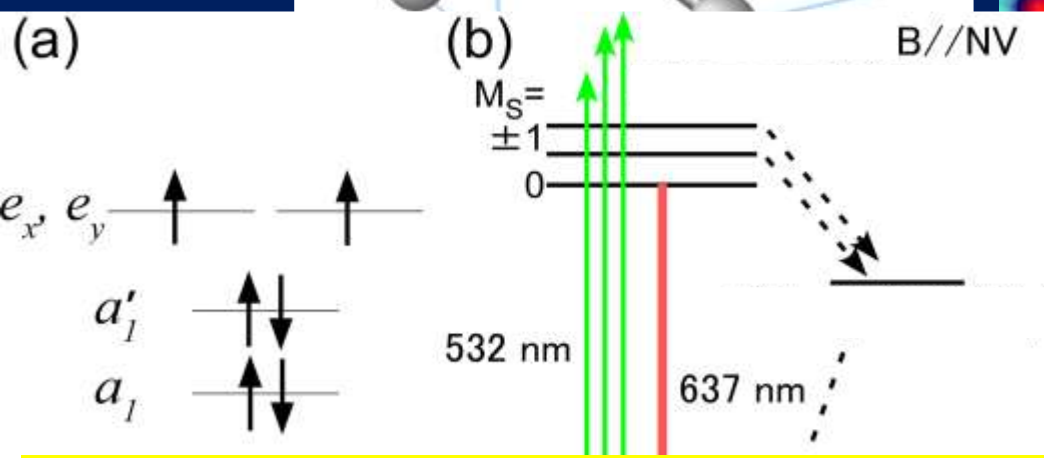
Nature 2006, News and Views

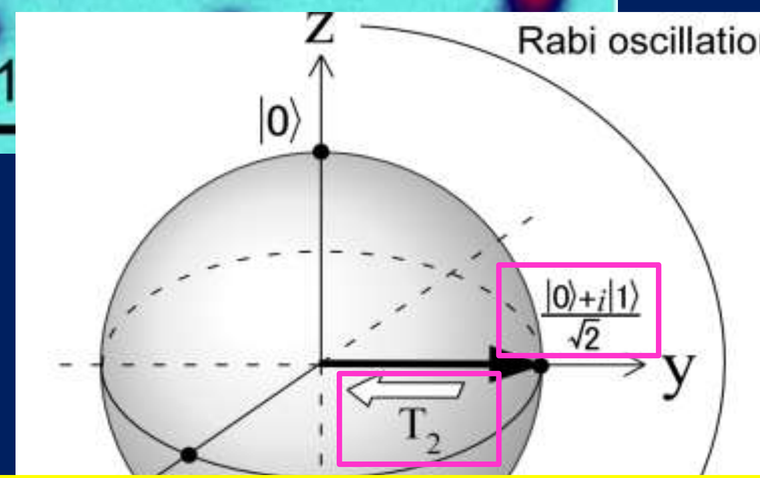
According to materials scientist F. Franck, "crystals are like people; it is only the defects that make them interesting".

NV center in diamond









Coherent Control and detection of Single spin at RT

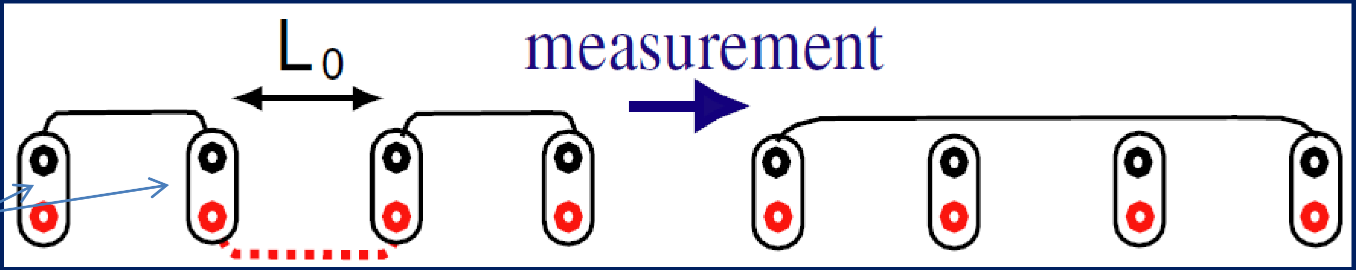
Unique character among solid state material

Quantum Cryptography

BB84: completely secure communication
by using single photon

Single photon source, Quantum repeater
("spin" for processing and memory, "Photon" for communication)

Quantum Repeater

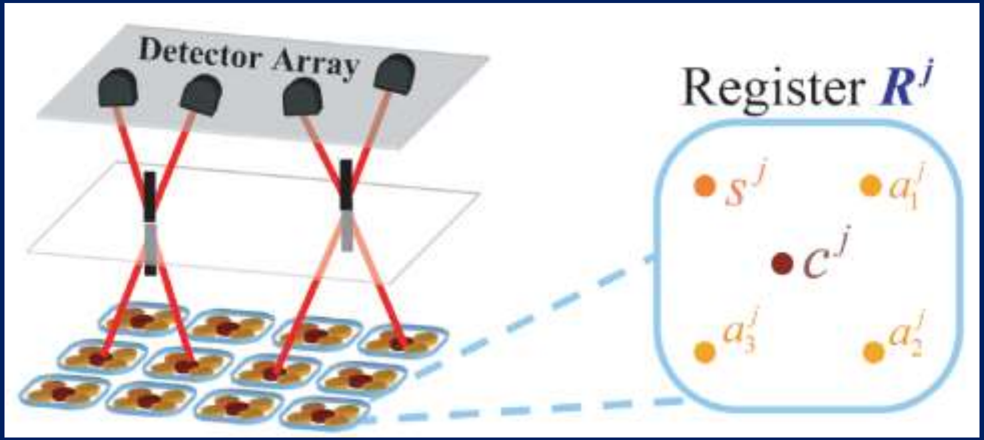


Black and Red ball represent spins (Qubits).

L. Childress, et al., PRL 2006.

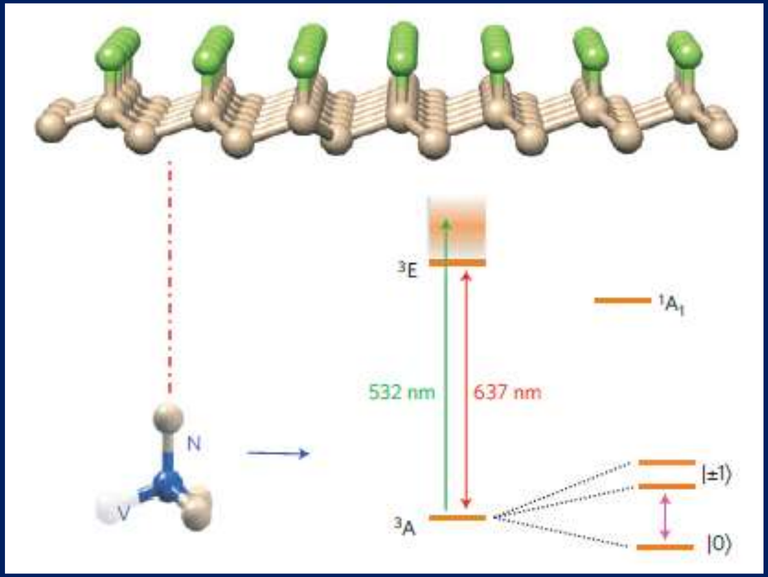
Quantum Computing

Distributed scalable quantum computer



It consists of 5 qubits quantum registers.
Jiang et al., PRA 2007

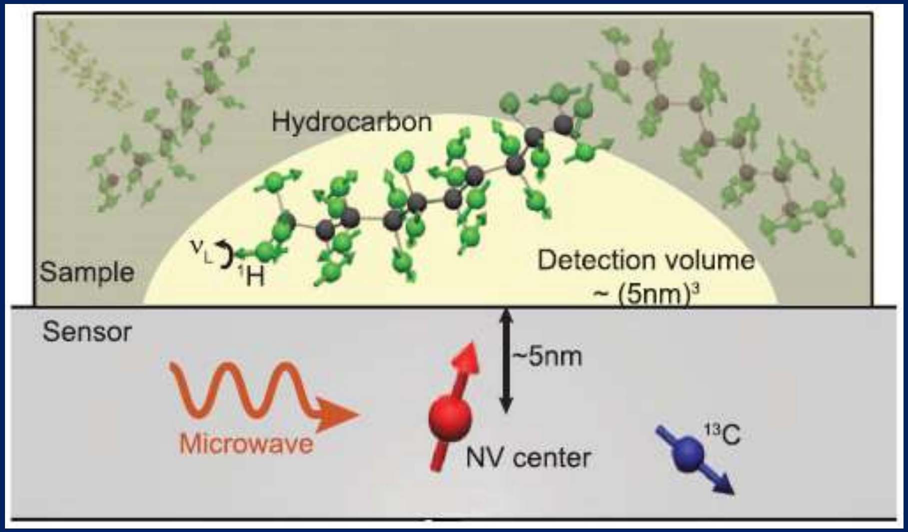
Quantum Simulation



Quantum simulation by NMR on the diamond surface: Initialization and readout is carried out by NV center
Cai et al., Nat. Commun. 2014

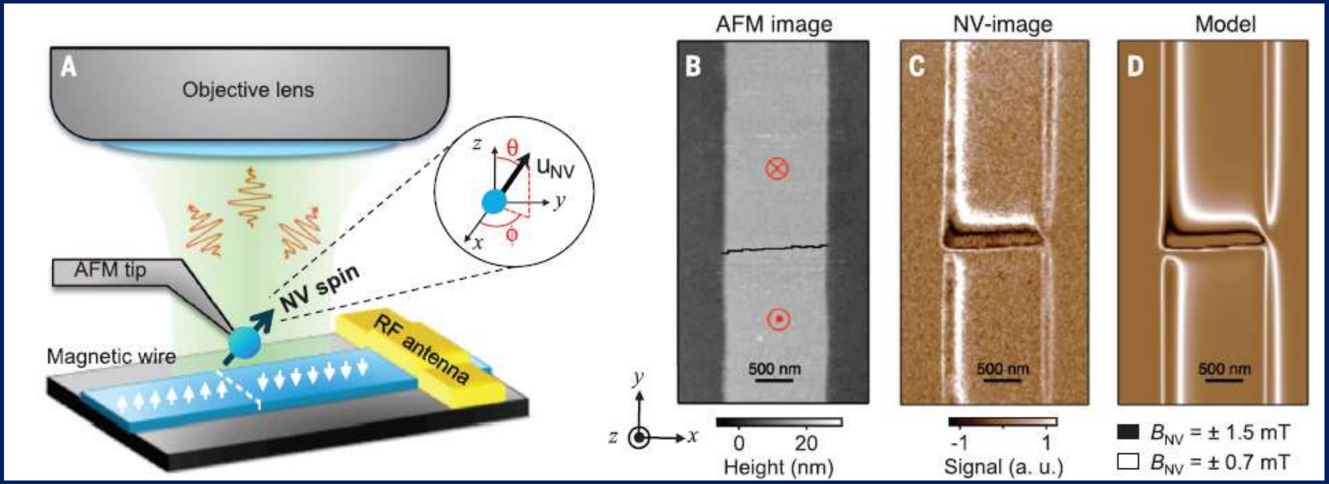
Sensor (Magnetic, Electric field, Temperature…)

High resolution and high sensitive sensor



NMR of molecules on diamond surface

Science 2013



Nanoscopy of domain walls

Science 2014

Scanning probe magnetometry (magnetic sensor)

Minimum detectable magnetic field

$$\delta B \simeq \frac{1}{g_s \mu_B} \frac{1}{R\sqrt{\eta}} \frac{1}{\sqrt{NtT_2^*}},$$

R: Measurement contrast
η: detection efficiency
N: number of spin centers
t: integration time

Single (RT)

B_{AC}=4.3 nT $Hz^{-1/2}$

Nature Mat. 2009

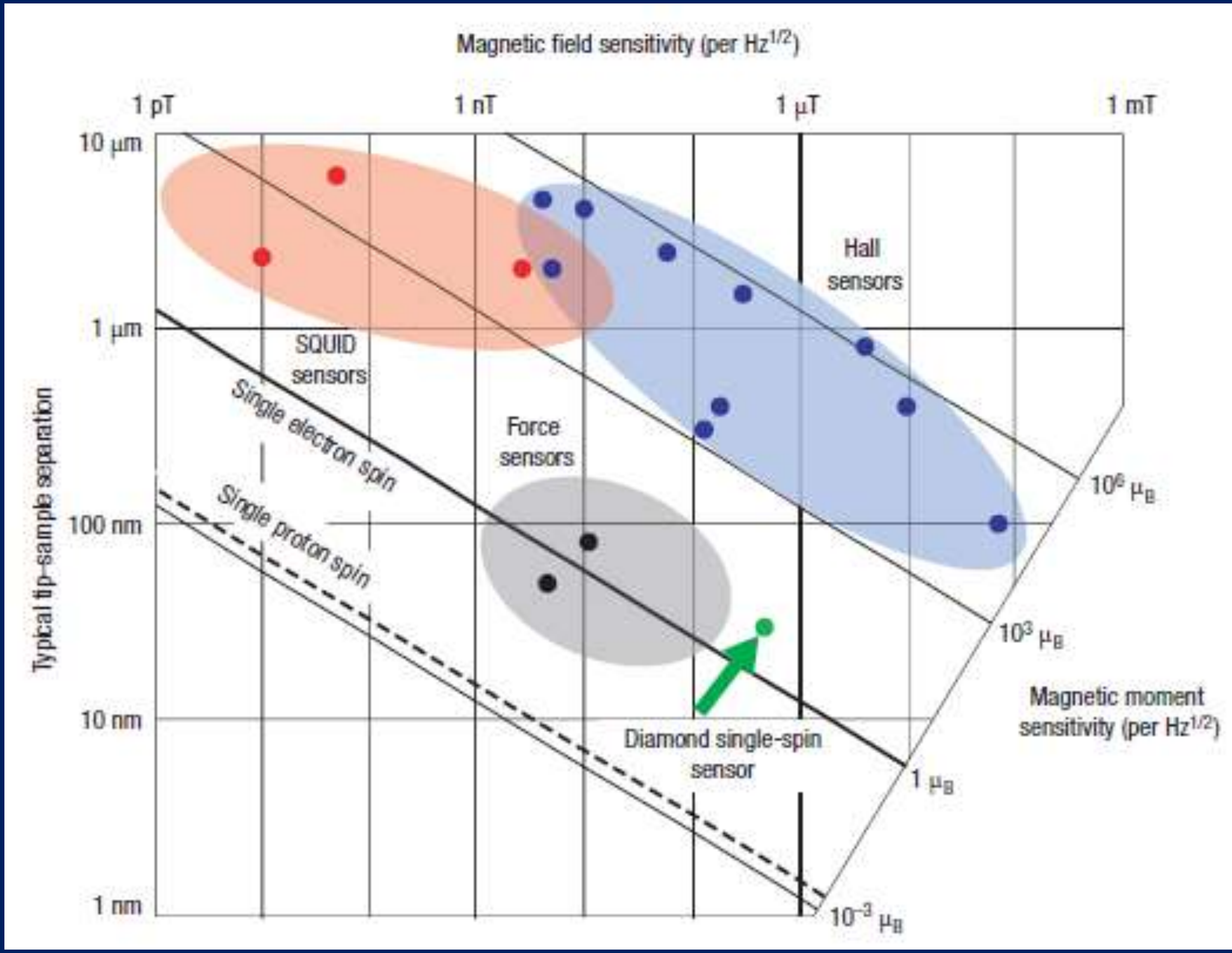
B_{DC}=0.3 μT $Hz^{-1/2}$

PRB 2009

Ensemble (RT)

B_{AC}=~ 100 pT $Hz^{-1/2}$

PRB 2012



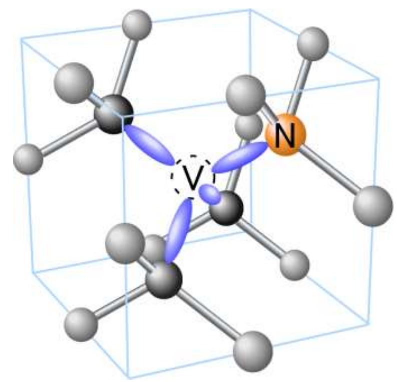
C. Degan, Nature nanotechnology, 3, 643 (2008).

The previous and recent our researches

Quantum hybrid system with superconducting flux qubit
Nature 2011, Nature commun. 2014
Collaboration with NTT, NII

Spin

QIP by single spins
Science 2008,
Nature Materials 2009,
PRB 2009



Electrical control of charge state
PRX 2014

Quantum Opt-spintronics

Charge

Photon

Electrically driven single photon source
Nature Photonics 2012

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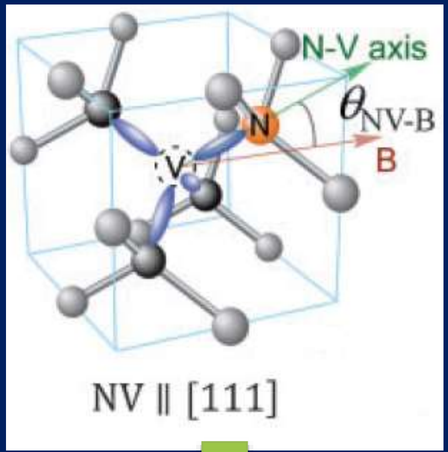
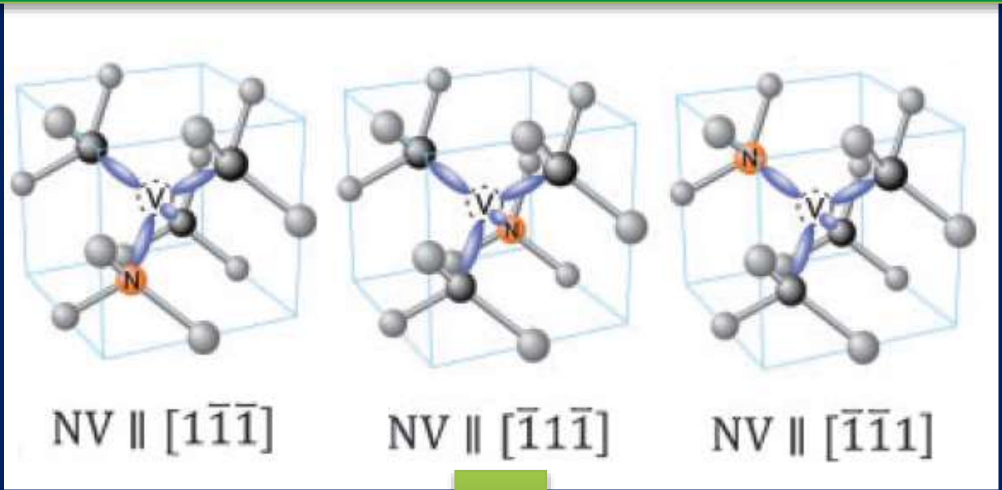
   T. Miyazaki, NM, et al., *Appl. Phys. Lett.* 105, 261601 (2014).

Magnetic field sensor sensitivity





the readout signal

the background signal

Magnetic field sensitivity (Minimum detactable B) : η

$$\eta \propto \frac{1}{C\sqrt{n_{NV}\,\tau\,T_2}}$$

C : readout contrast

n_{NV}: The number of NV

τ : Measurement time

L. M. Pham, et. al., Phys. Rev. B **86**, 121202 (2012)

η Four-fold enhancement due to four possible orientation

It is important to control NV orientation for magnetic sensor

Advantage of perfect alignment

1. Improvement of sensitivity (four times)

$$\eta \propto \frac{1}{C\sqrt{n_{NV}\tau T_2}}$$

C : readout contrast

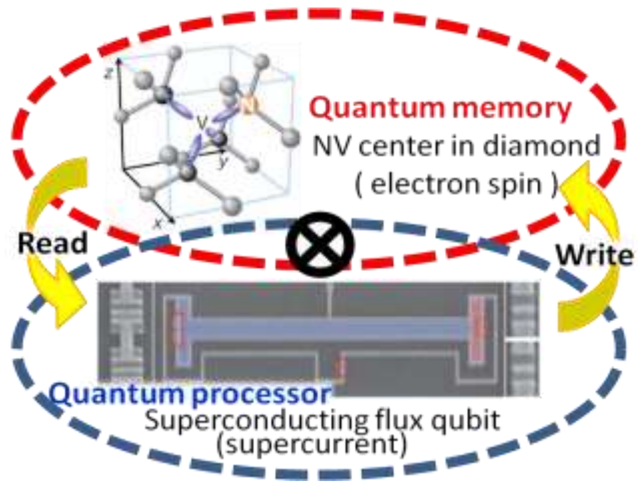
n_{NV}: The number of NV

τ : Measurement time

T_2 : Coherence time

L. M. Pham, et. al., PRB **86**, 121202 (2012)

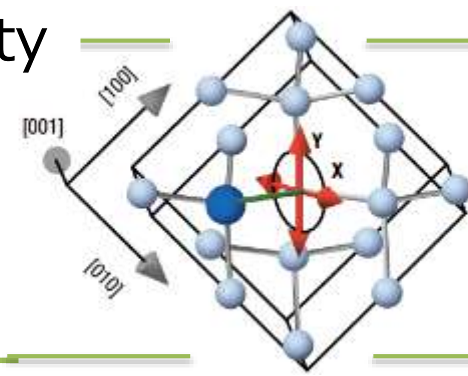
2. Extension of T_2



X. Zhu, et. al., Nature **478**, 221 (2011)

3. Improvement of luminescence intensity

Electric dipole transitions are in the plane perpendicular to the N–V axis.

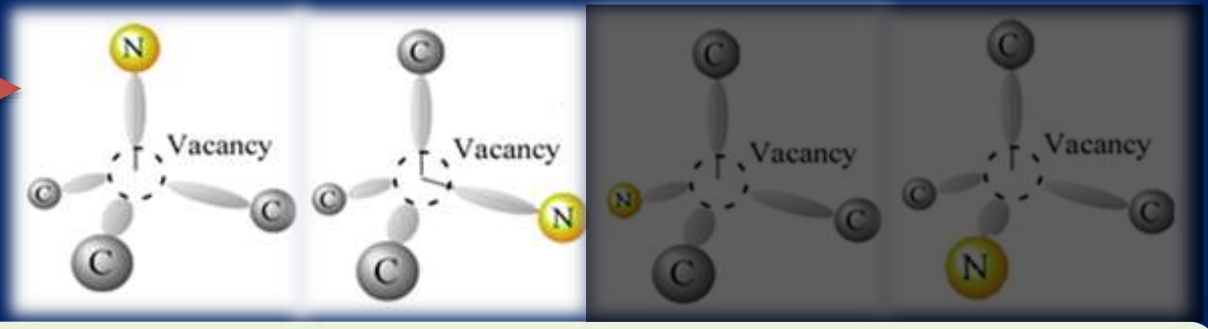


R. J. Epstein, et al., *Nature Physics* **1**, 94 - 98 (2005)

Previous researches on (110), (100)

CVD layer

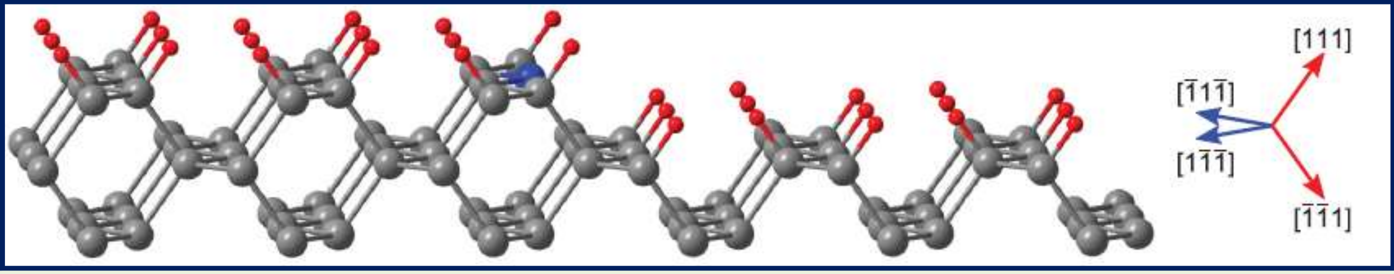
(110) and (100) diamond substrate



NV aligned along two of the four orientation in (110)- CVD diamond.

A. M. Edmonds, et. al., Phys. Rev. B **86,** 035201(2012)

Preferential orientation along only [111] and [-1, -1, 1] directions



NV aligned along two of the four orientation in (100)- CVD diamond. The readout contrast and magnetic field sensitivity can be enhanced by a factor of two.

$$\eta \propto \frac{1}{C\sqrt{n_{NV}\tau}}$$

L. M. Pham, et. al., Phys. Rev. B **86,** 121202 (2012)

Recent researches

Independent three groups reported perfect alignment (selective alignment of one of four orientation) in (111) CVD diamond simultaneously at around March 2014.

- J. Michl, et al., Appl. Phys. Lett. 104, 102407 (2014).
- M. Lesik, et al., Appl. Phys. Lett. 104, 113107 (2014).
- T. Fukui, NM, et al., Appl. Phys. Express 7, 121202 (2014).

T. Miyazaki, NM, et al., Appl. Phys. Lett. 105, 261601 (2014).

Angular dependence of resonance

Spin Hamiltonian of NV center under magnetic field (B)

$$\mathscr{H}_S = DS_z^2 + E(S_x^2 - S_y^2) + g_s\mu_B\vec{B}\cdot\vec{S}$$

D, E : zero field splitting parameter
gs : electron g-value
μB : Bohr magneton

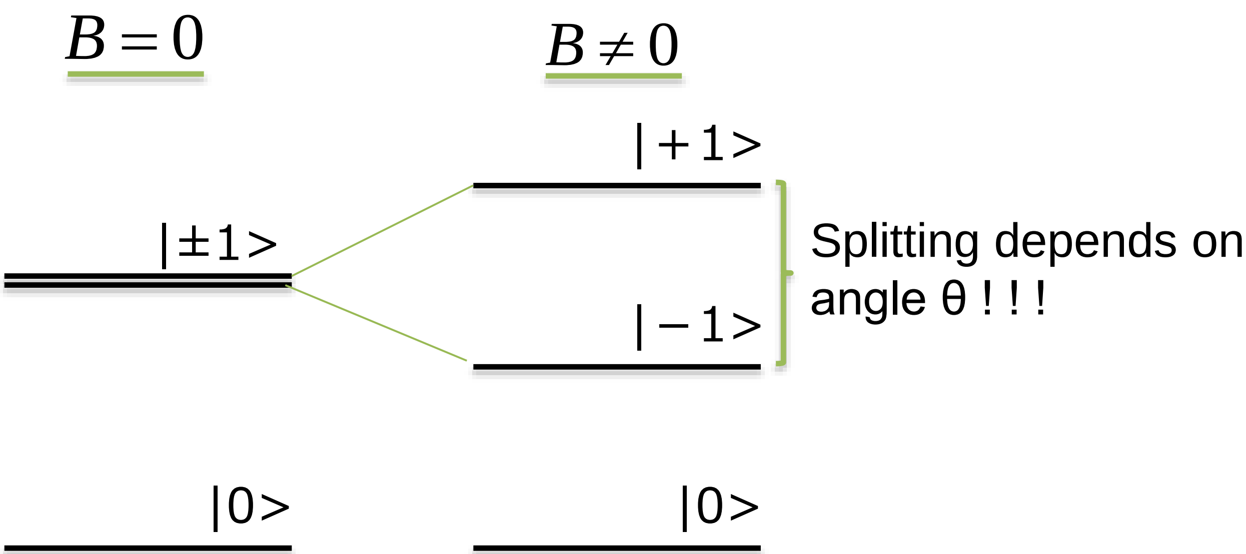
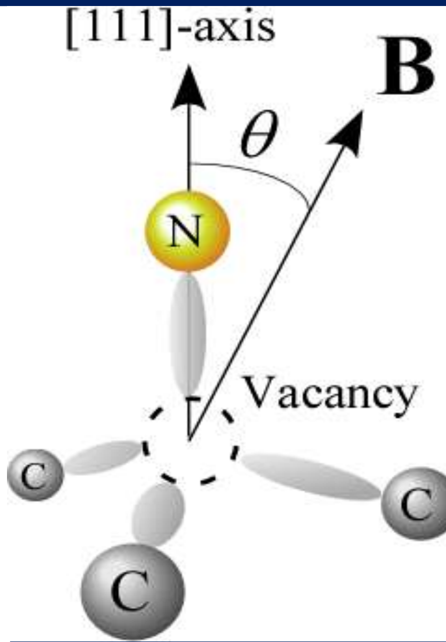


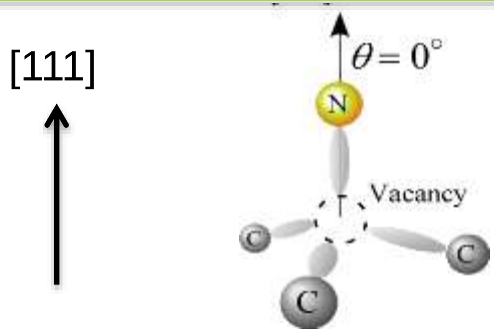
Fig. electronic spin structure of ground state of NV center

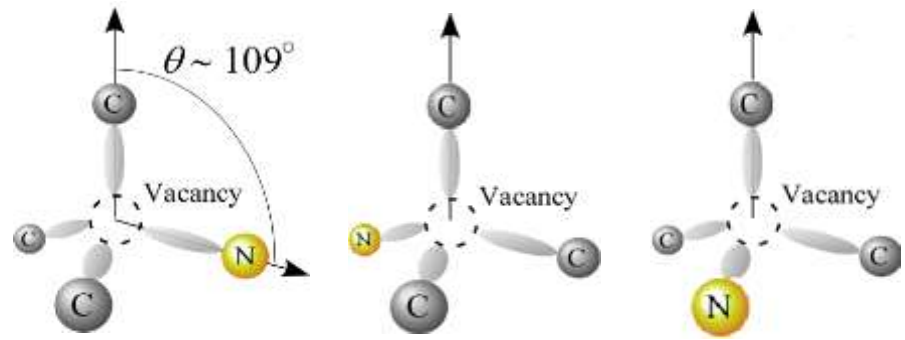


Splitting width depends on angular θ between the direction of NV axis and magnetic field

Investigation of the NV orientation by ESR

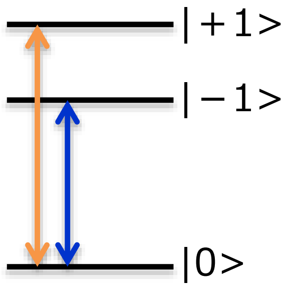
In the case of B//[111]



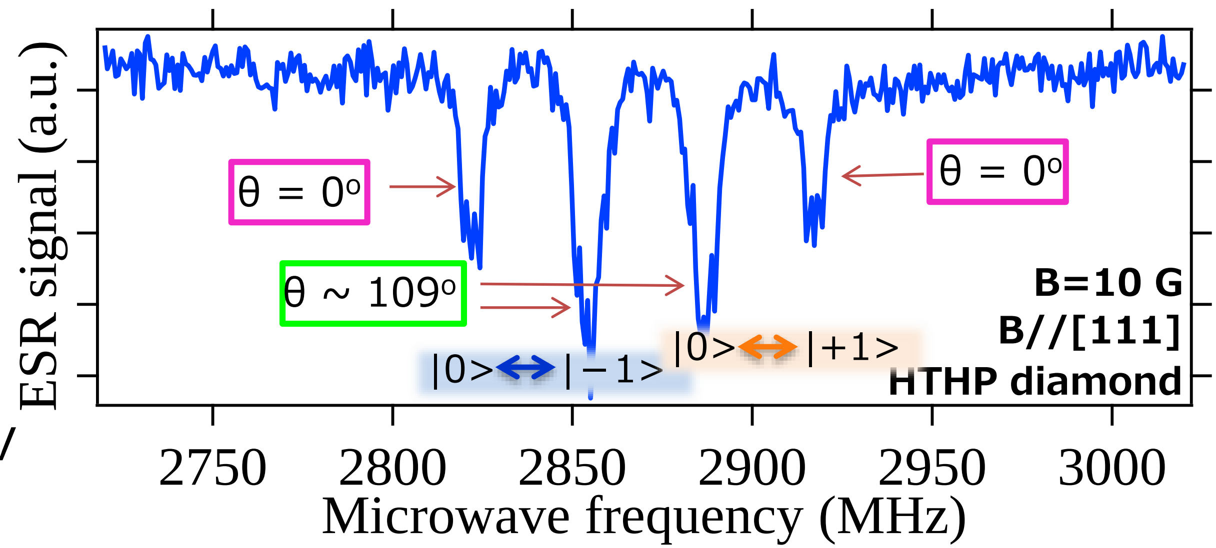


When NV orientation is along [111] direction, $\theta = 0°$

When NV orientation is along except for [111] direction, $\theta \sim 109°$



Electronic spin structure of NV center under B



Assignment of the NV orientation by magnetic resonance

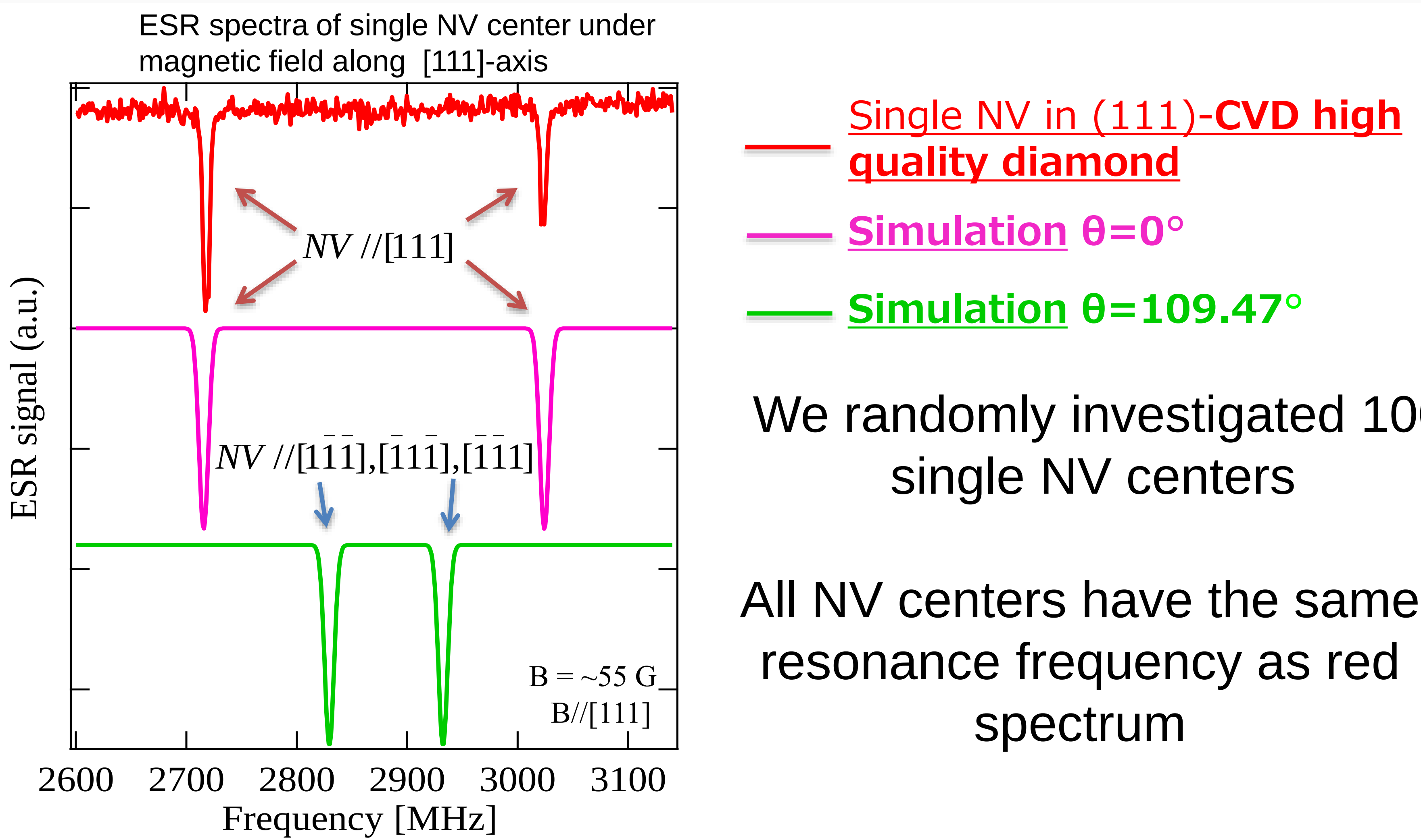
CVD growth condition

- Epitaxially deposited on HPHT synthetic Ib diamond (111) substrates.
- Nitrogen was unintentionally incorporated during CVD growth.

	single	ensemble	3D
Chamber	ASTeX	ARIOS	ARIOS
MW power (W)	3500	400	800
CH_4/H_2	0.25	0.15~0.25	4
Temp. (deg C)	850	900	1100
Growth rate (micron/hour)	5.5	4.8	38

High quality

Measurement result ~single ~



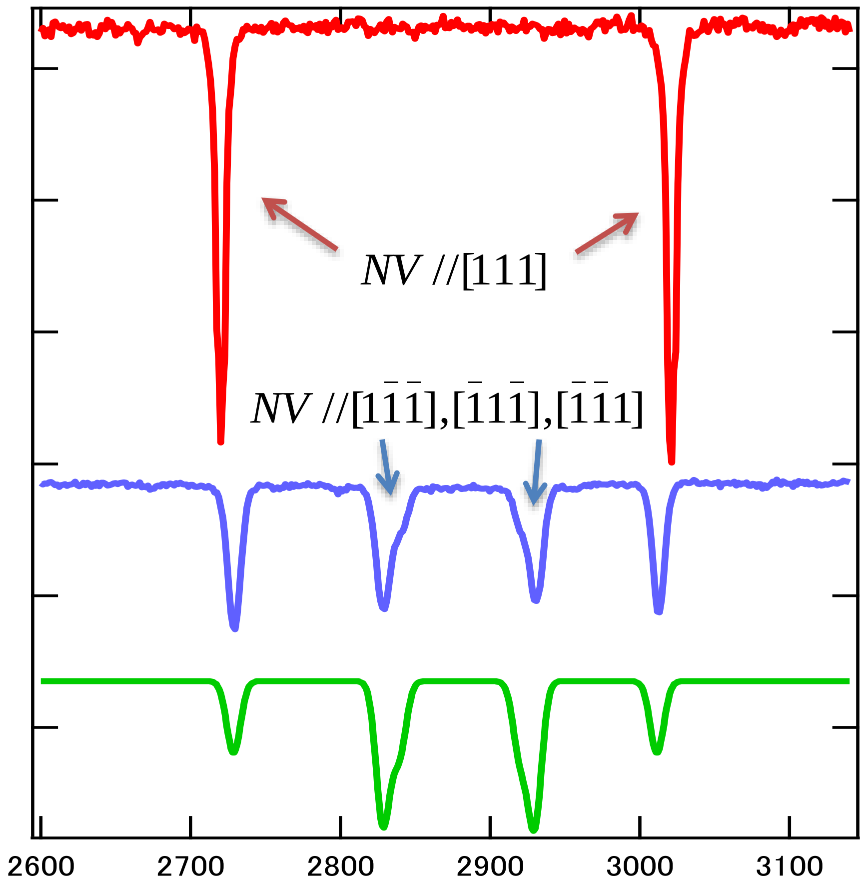
We randomly investigated 100 single NV centers

All NV centers have the same resonance frequency as red spectrum

The orientation of more than 99% of the single NV centers in (111)-CVD diamond were aligned along the [111] axis

Measurement result ~ensemble ~

Fig. ODMR spectra of ensemble NV centers under magnetic field along [111]-axis



in (111)-**CVD high quality diamond**

in (111)-**HTHP diamond**
(NV is incorporated by e-irradiation)

Simulated blue spectrum

Only two peaks NV//[111] appear !

We randomly investigated more than 10 locations

All NVs exhibit an NV//[111] orientation

We show the orientation of ~99% of the NV centers in (111)-CVD diamond can be aligned along the [111] axis

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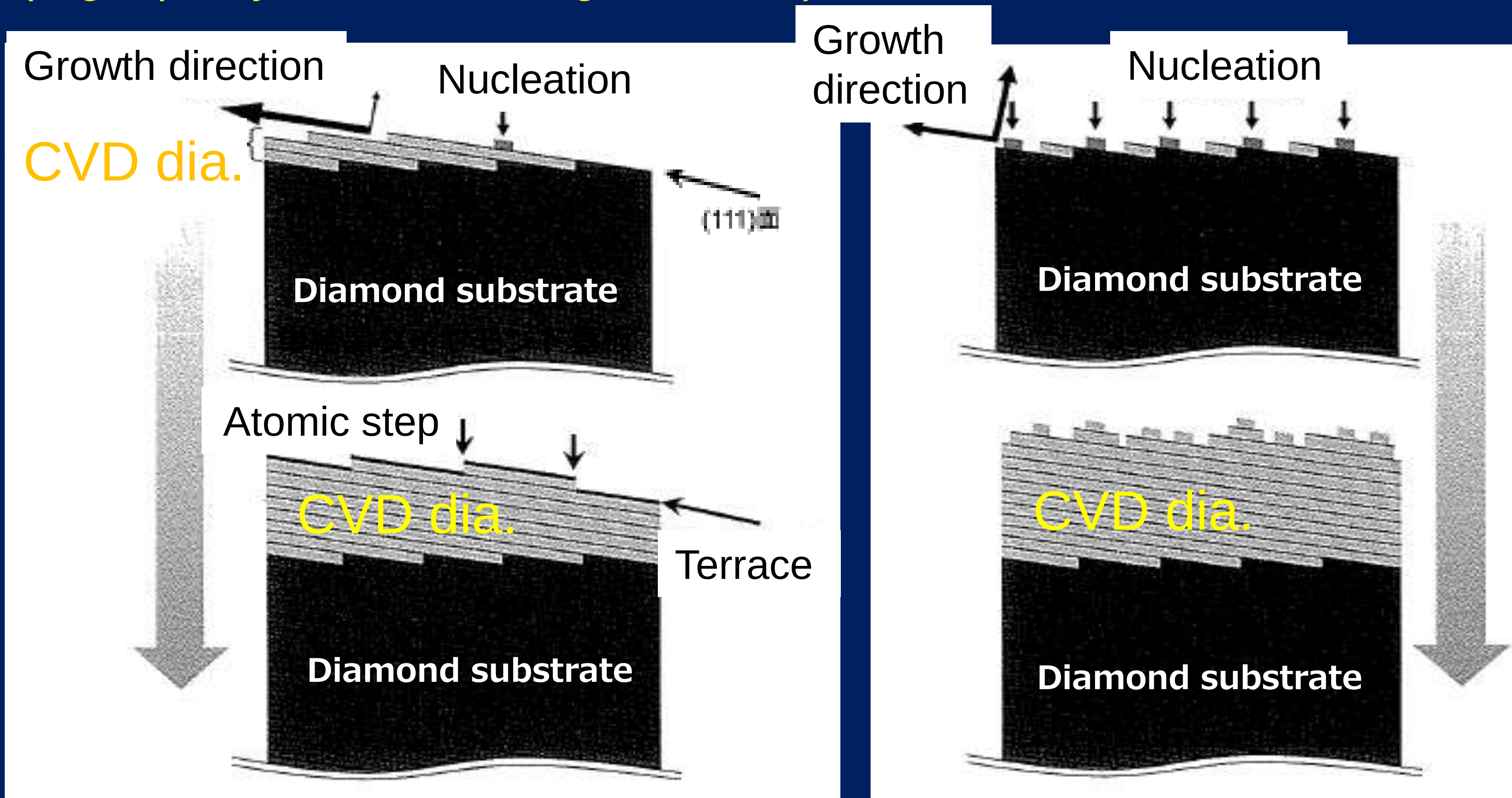
Growth of CVD diamond and orientation ratio

Two dimensional island growth
(High quality diamond: low growth rate)

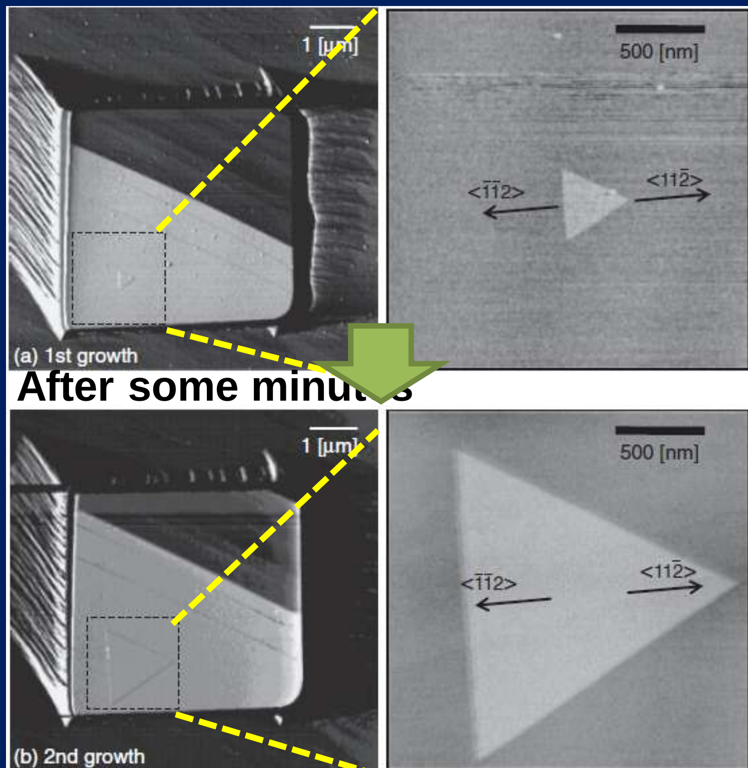
Three dimensional growth
(High growth rate)



We investigated dependence on growth mechanism.

(111)-CVD diamond growth ~Kink flow~

How to grow (111)-diamond by CVD

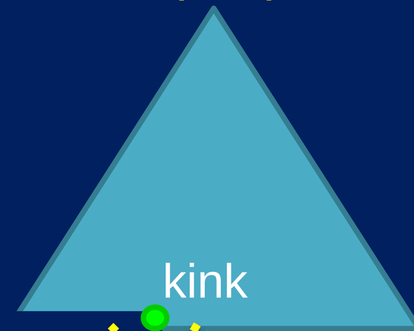


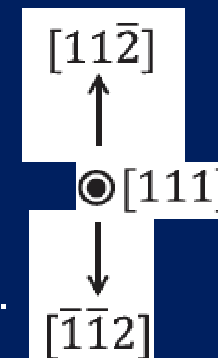
AFM image of diamond surface

Step-down direction is [-1, -1, 2]

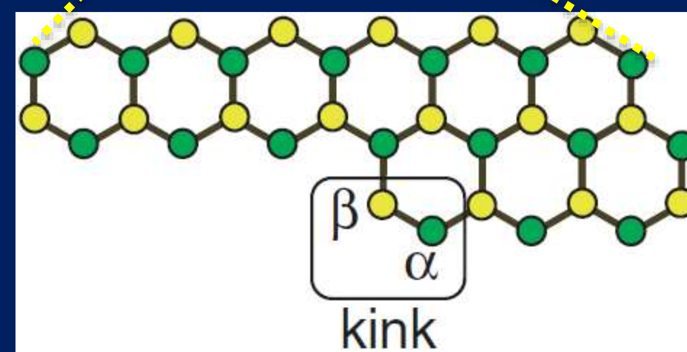
N. Tokuda, et al., Jpn. J. Appl. Phys. (2014)

kink flow of (111)-diamond island





Diamond growth occur at kink.



(111)- diamond bi-layer structure

α site is the top C atom in bi-layer

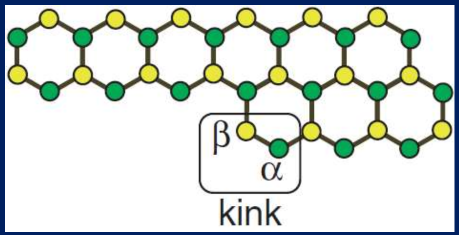
β site is the second C atom in bi-layer

(111)-diamond grows by C atom incorporation to α and β site in kink

Theoretical study

We calculated which N is energetically favorable (at α or β site?)

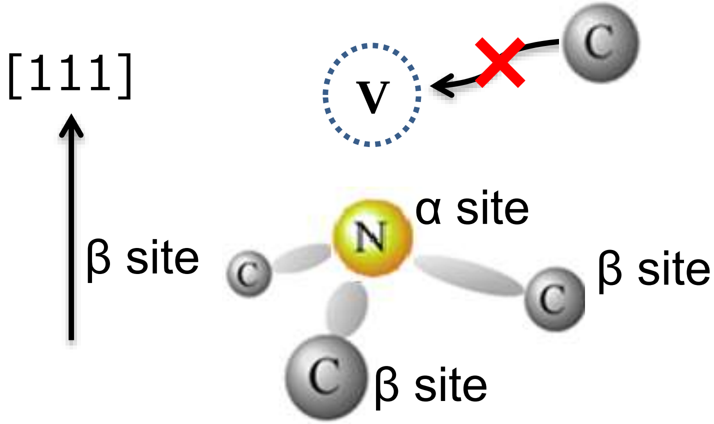
(With first-principles calculation)



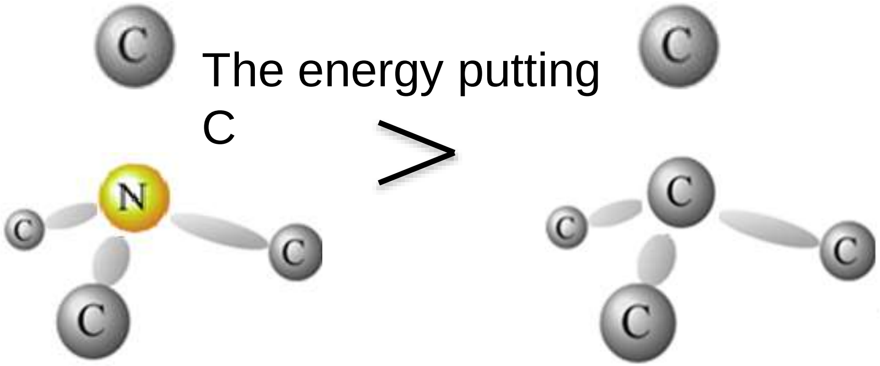
The N at the α kink site is energetically favorable.

(0.51 eV)

When an N atom is incorporated at α site



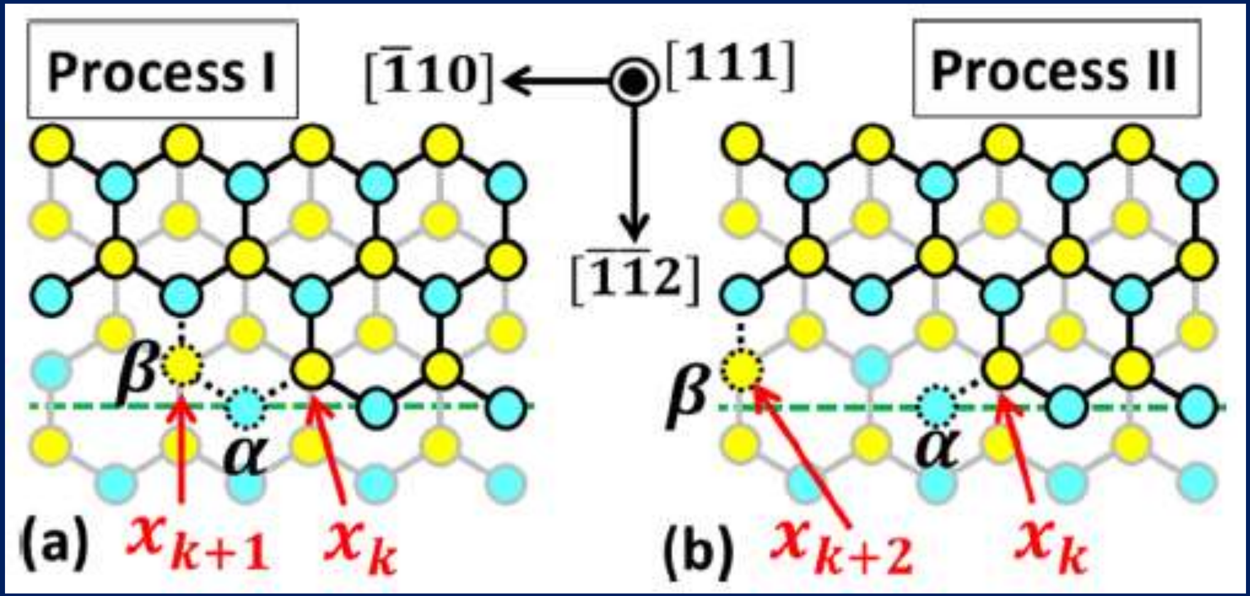
N atom has lone pair.
So, C is difficult to put on N atom



The energy putting C on N atom is larger (3 eV) than ones on C itself

First-principles calculation

T. Miyazaki, NM, et al., *Appl. Phys. Lett.* 105, 261601 (2014).



- Two elementary processes of kink flow were considered.
- In process I, two carbon atoms are attached to the kink at x_k.
- Then the x_{k+1} site forms a new kink.
- In process II, a C atom occupies the β site at x_{k+2} while the other C atom as process I. The process II creates a vacancy.

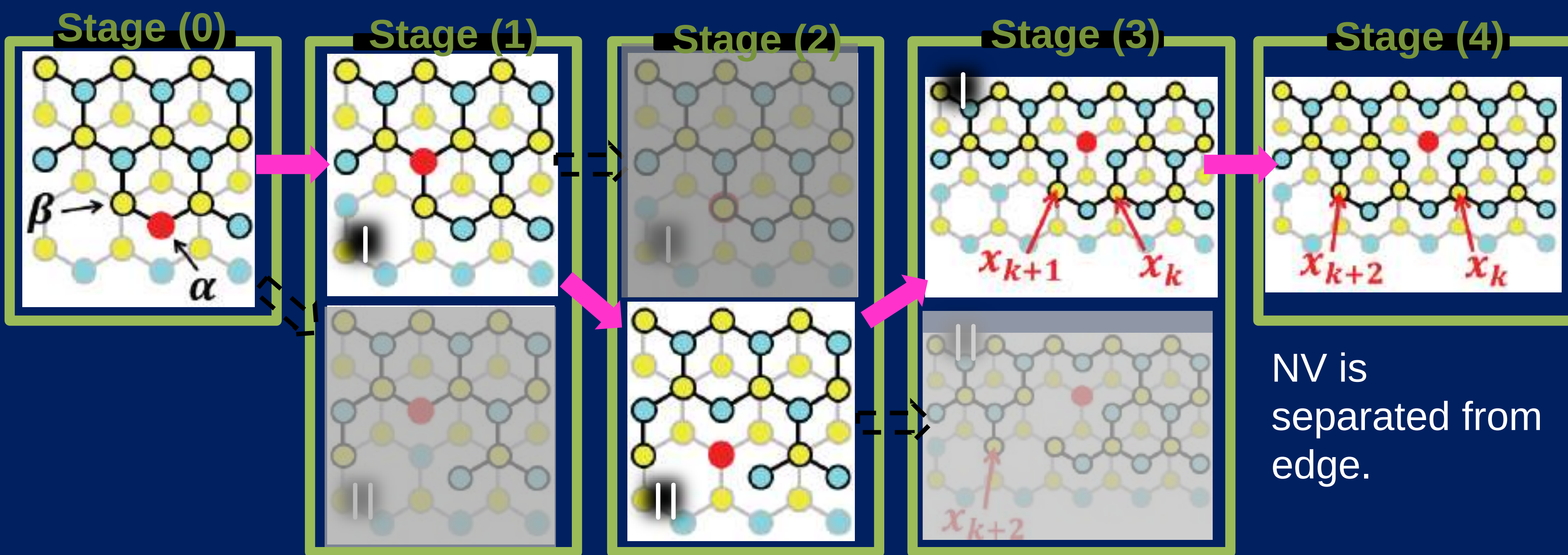
Total energies of structures

First principle electronic structure calc. based on DFT

T. Miyazaki, NM, et al., *Appl. Phys. Lett.* 105, 261601 (2014).

-2.3 eV

-0.3 eV



NV is separated from edge.

N: at kink

N: Surface terrace

C bilayer is overgrown

NV is embedded in second bilayer.

-1.6 eV

Our theoretical scenario explains the results.

Summary

- The orientation of more than 99% of the NV centers could be aligned along the [111] axis by high quality growth technique.
- The atomistic mechanism was examined and explains the results.

T. Fukui, NM, et al., *Appl. Phys. Exp*. 7, 055201 (2014), selected in "Spotlights"
T. Miyazaki, NM, et al., *Appl. Phys. Lett*. 105, 261601 (2014).

Important in application for quantum information, sensing, …