Germanium Detector Passivation Techniques

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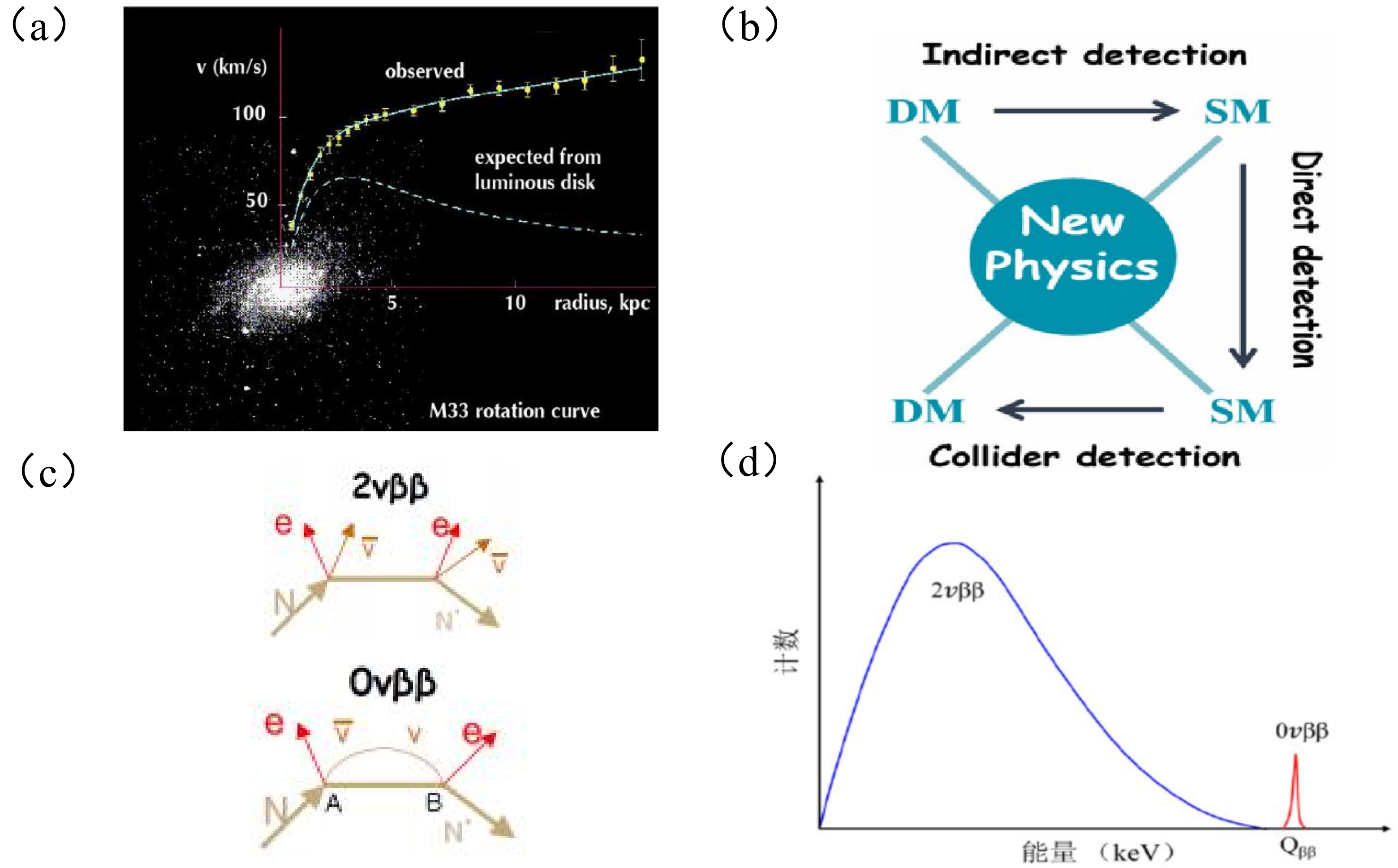
PIRE GEMADARC Collaboration Meeting Agenda, June 1&2 , 2023

Content

Rare event detection



(a) Evidence for dark matter: galaxy rotation curve, (b) method for dark matter detection, (c) 2vββ and 0vββ Feynman diagram；（d）Possible energy of 0vββ[1,2]

Implications for dark matter detection：

- Dark matter **plays an important role** in the formation and evolution of the universe
- Involves research topics such as **elementary particles**

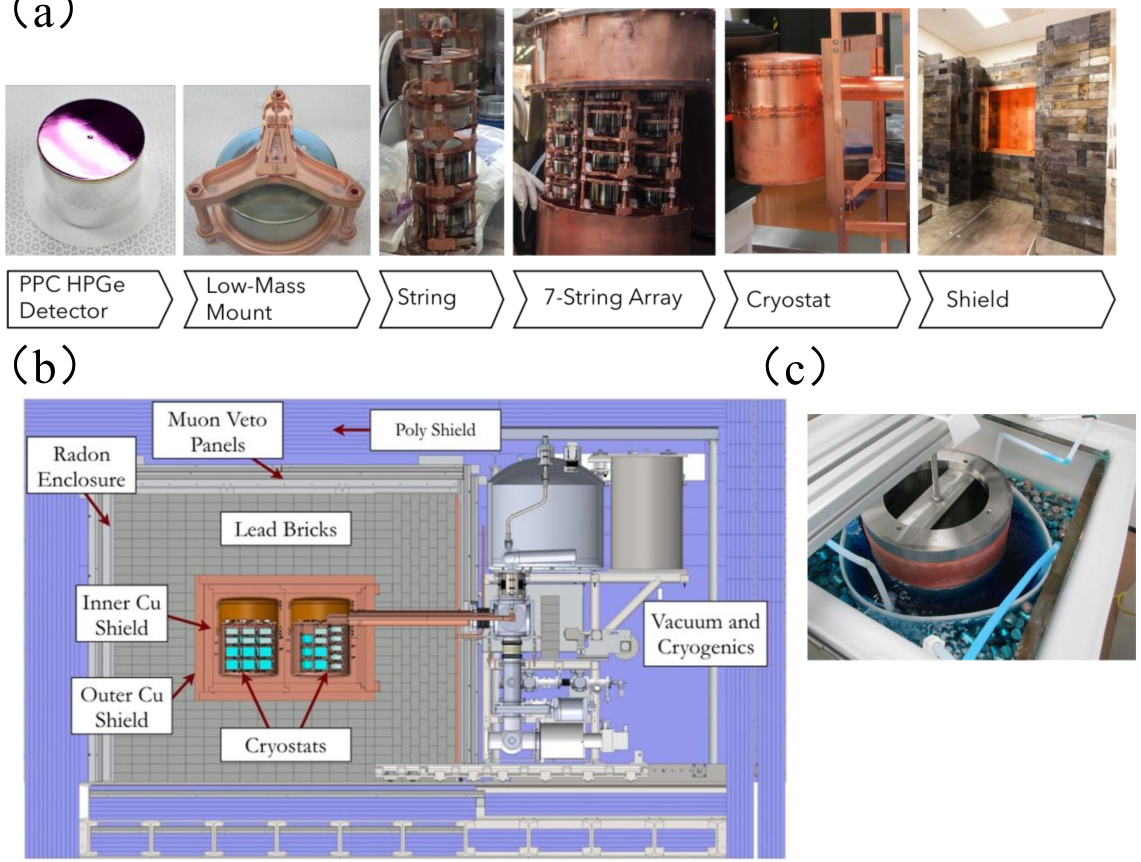
Implicaions for *0vββ* detection：

- Neutrino mass order
- The **only viable way** to prove whether neutrinos are their own antiparticles is to be neutrinos,
- Understanding the **neutrino mass origin problem**

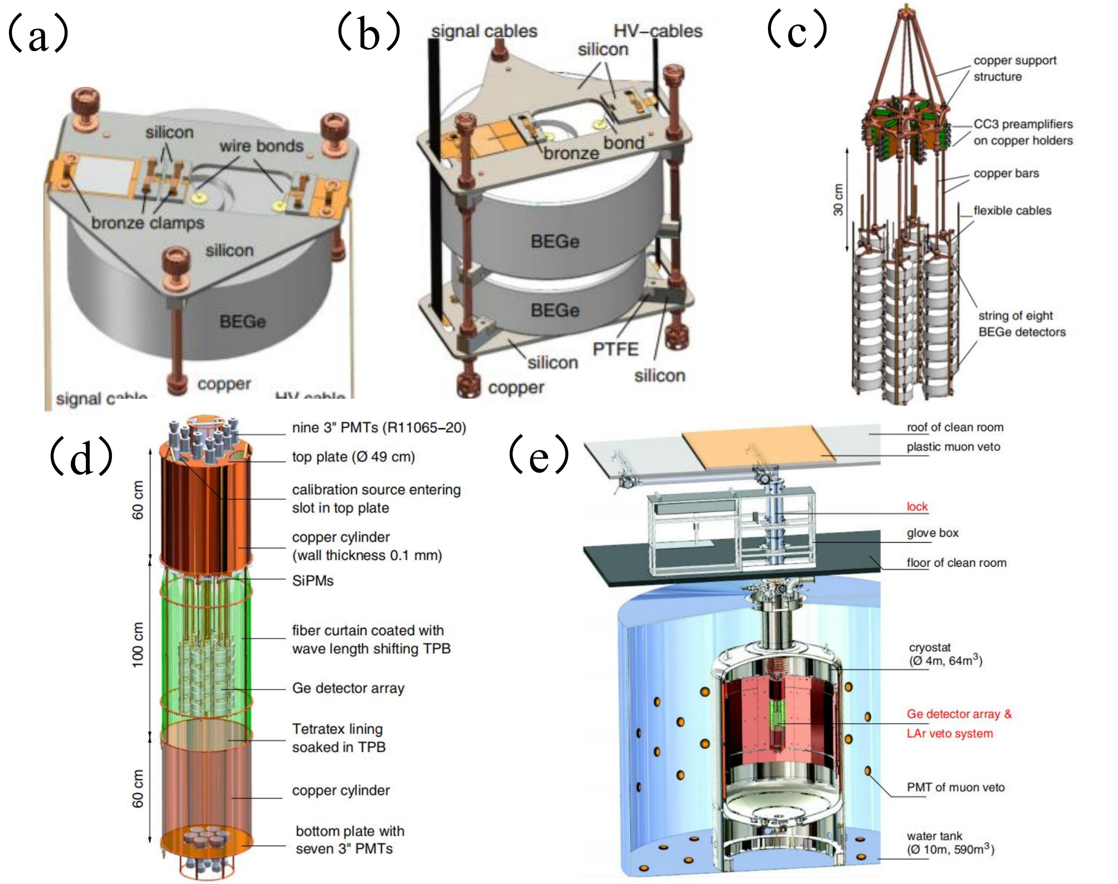
[1] Zwicky F. Die rotverschiebung von extragalaktischen nebeln[J]. Helvetica physica acta, 1933, 6: 110-127.
[2] ROSZKOWSKI L, SESSOLO E M, TROJANOWSKI S. WIMP dark matter candidates and searches-current status and future prospects[J]. Reports on Progress in Physics Physical Society (Great Britain), 2018, 81(6): 066201

Rare event detection

Direct detection method **HPGe detecrors**



Schematic diagram of MAJORANA experimental apparatus: (a) the composition of HPGe array, (b) shieding device diagram； （c）MAJORANA experimental characteristcis：underground electroforming copper[1]

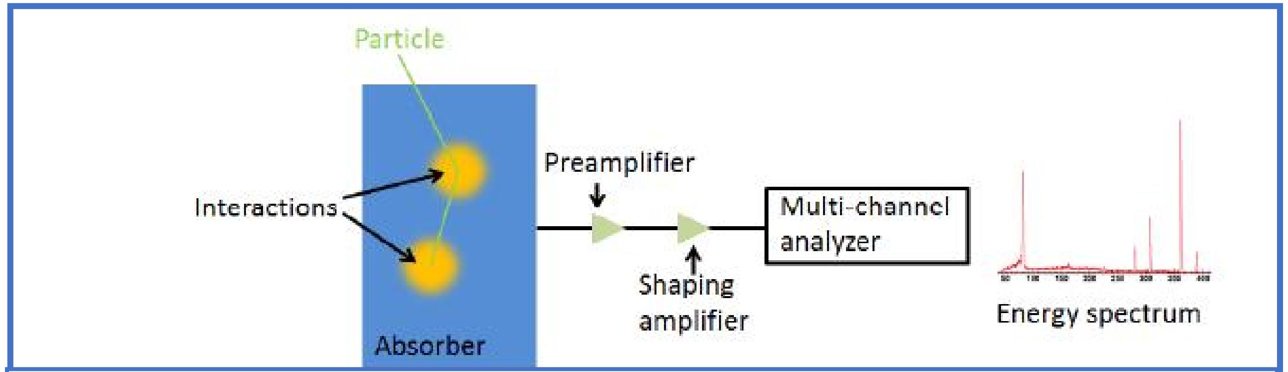


Schematic of GERDA experimental apparatus: (a) Single BEGe fixing device diagram, (b) BEGe array, (c) Seven string high BEGe array, (d) GERDA experimental liquid argon anticoincidence device, (e) Schematic diagram of GERDA Phase II experimental device [2]

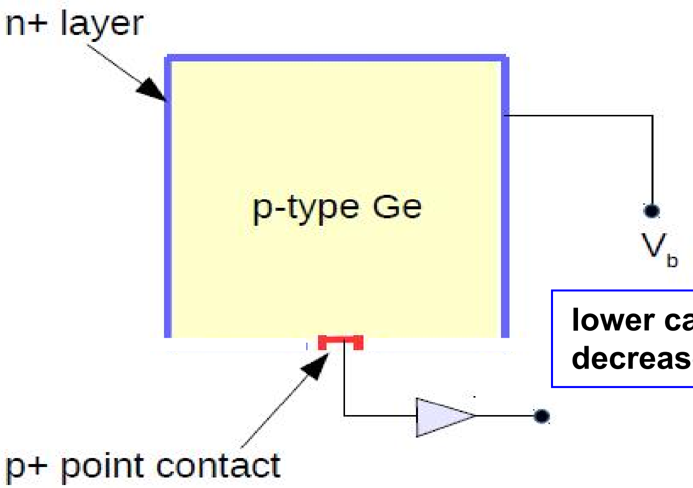
[1] N. Abgrall，I. J. Arnquist，F. T. Avignone III et al. The processing of enriched germanium for the MAJORANA DEMONSTATOR R&D for a next generation double-beta decay experiment[J]. NUCLEAR INSTRUMENTS AND METHODS IN PHYSICS RESEARCH SECTION A，2018
[2] AGOSTINI M, ARAUJO G R, BAKALYAROV A M, et al. Final results of GERDA on the search for neutrinoless double-β decay[J]. Physical Review Letters, 2020, 125(25): 252502

HPGe detecrors

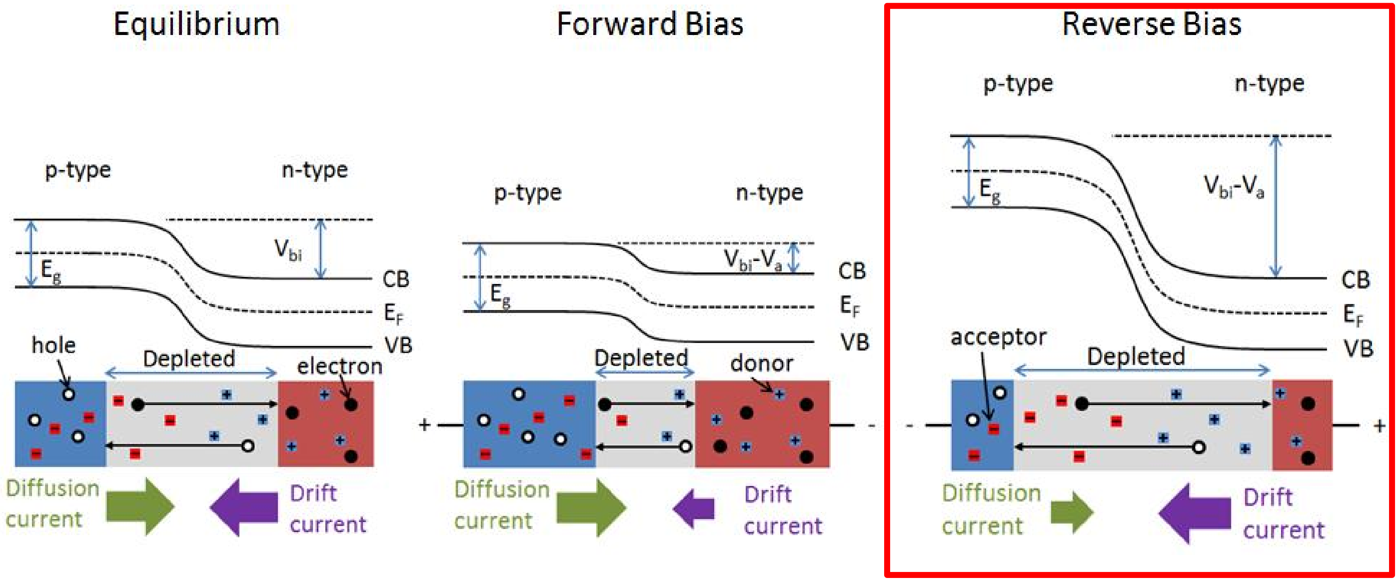
Energy resolution (0.2% FWHM at 662keV), **linear energy response, lower energy threshold**

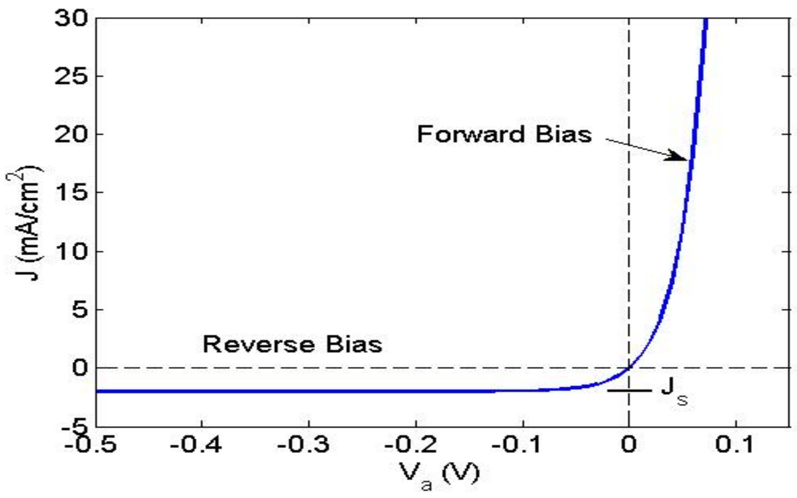


Basic components of radiation detection system



lower capacitance
decrease electronic noise



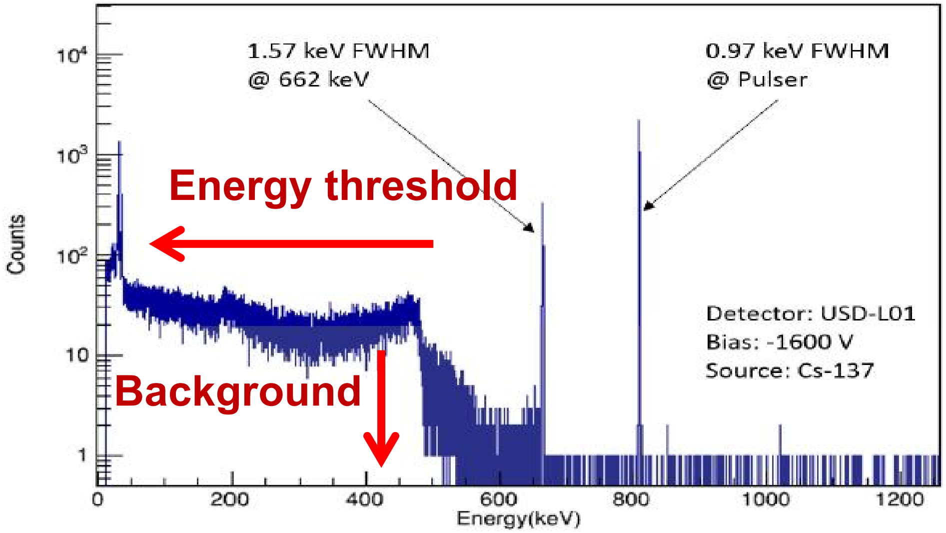


HPGe detecrors

Small band gap
Free carrier concentration of 10^{13} /cm^3 at RT, 10^9 /cm at 77 K
High activated carrier leakage current at RT

Material	Bandgap at 300 K (eV)	e-h pair creation energy (eV)	Density (g/cm^3)	Mean Z
Si	1.12	3.6	2.33	14
Ge	0.67	2.96	5.33	32
$Cd_{0.9}Zn_{0.1}Te$	1.57	4.64	5.78	49.1

Material	Hole mobility μ_h (cm^2/V·s)	Electron mobility μ_e (cm^2/V·s)	Hole lifetime τ_h (s)	Electron lifetime τ_e (s)	$\mu_h\tau_h$ (cm^2/V)	$\mu_e\tau_e$ (cm^2/V)
Ge (77 K)	42000 [43]	36000 [44]	2×10^{-4} [45]	2×10^{-4} [45]	>1 [31]	>1 [31]
Si (300 K)	450 [47]	1350 [47]	2×10^{-3} [46]	$>10^{-3}$ [46]	>1 [31]	>1 [31]
CZT (300 K)	30 [48]	1100 [48]	1×10^{-6} [46]	3×10^{-6} [46]	5×10^{-3} [2]	5×10^{-3} [2]



HPGe detecrors

Carrier injection current (77K is less than 1pA)

$$I_{tot} = AJ_{hi} + AJ_{ei} + I_{surf} + I_{bulk}$$

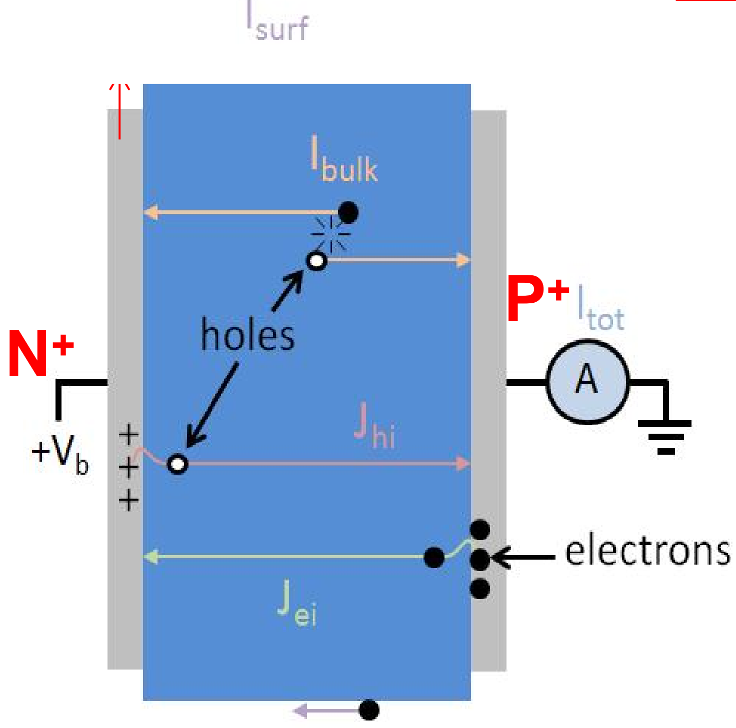
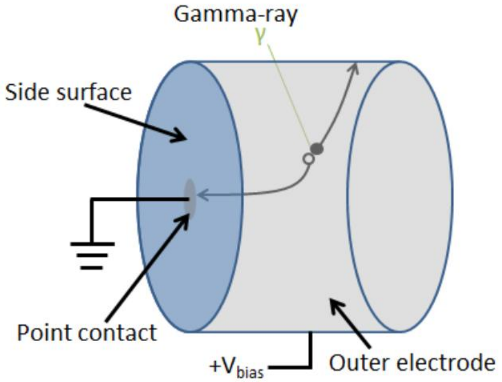


Table 3.3. Summary of key features for the different classes of electrical contacts on HPGe detectors.

Contact Type	Advantages	Disadvantages
Ion-implanted (B)	Thin, good electron blocking	No hole blocking, additional processing needed for segmentation
Li-diffused	Robust, good hole blocking	Thick, changes with time, transition region, difficult to segment, no electron blocking
Metal Schottky barrier	Thin, simple to construct, easily segmented, good electron blocking	Poor hole blocking, not robust, some lack of reproducibility
Amorphous semiconductor	Thin, blocks holes or electrons, doubles as passivation, easily segmented	Electron or hole blocking inferior to p-n junction, wide range of film properties

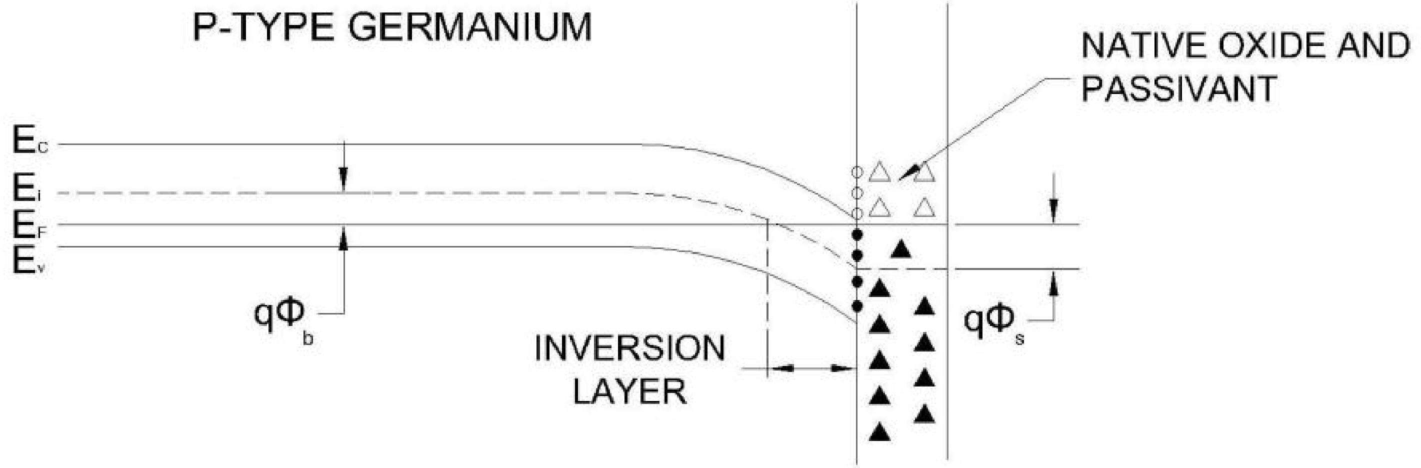


HPGe detecrors

Schottky Theory:

$$J=AT^2 e^{-\phi_B/kT}\,[e^{Va/kT}-1]$$

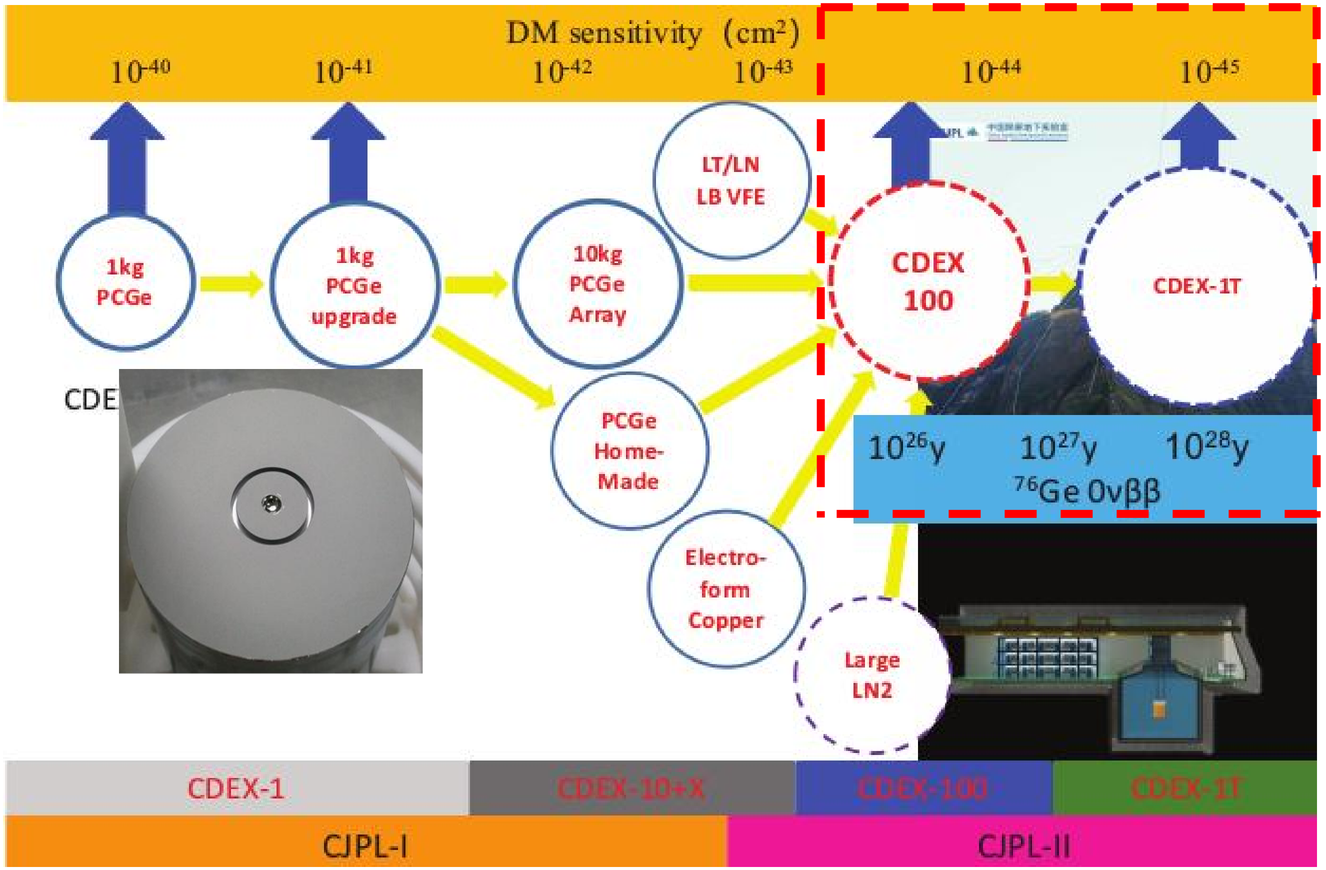
J: Saturation current under reverse bias
A：Richardson constant
ϕ_B: Interfacial potential barrier height



- The surface is sensitive to pollutants and water vapor, which changes the surface state and electric field distribution, make the surface charge collected.
- Surface suspension bond states and defects trap electrons and facilitate electron and hole separation, but also become the composite centers.
- Surface leakage current is generated.

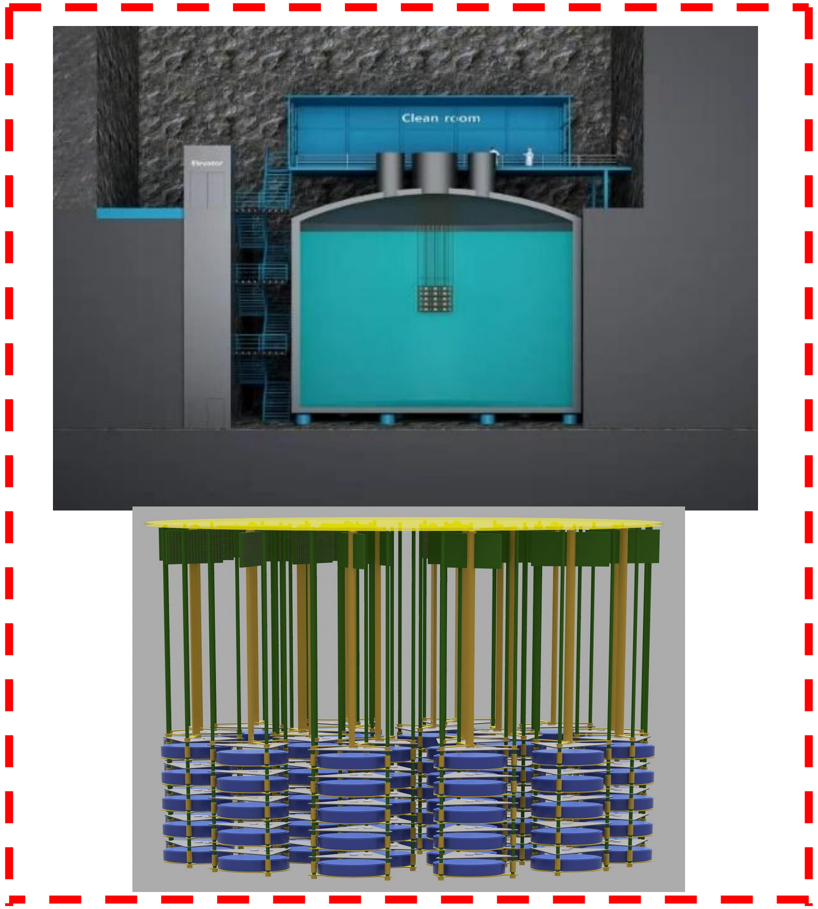
Avoid passivation layer charge collection
Avoid building up internal electric fields

CDEX experiments



CDEX experiment current and future plans[1]

Experimental design: liquid nitrogen or liquid argon liquid directly cooled HPGe detector array



CDEX expeirment future plans: experimental scheme adopted by 100 kg and 1 T HPGe detector array[1]

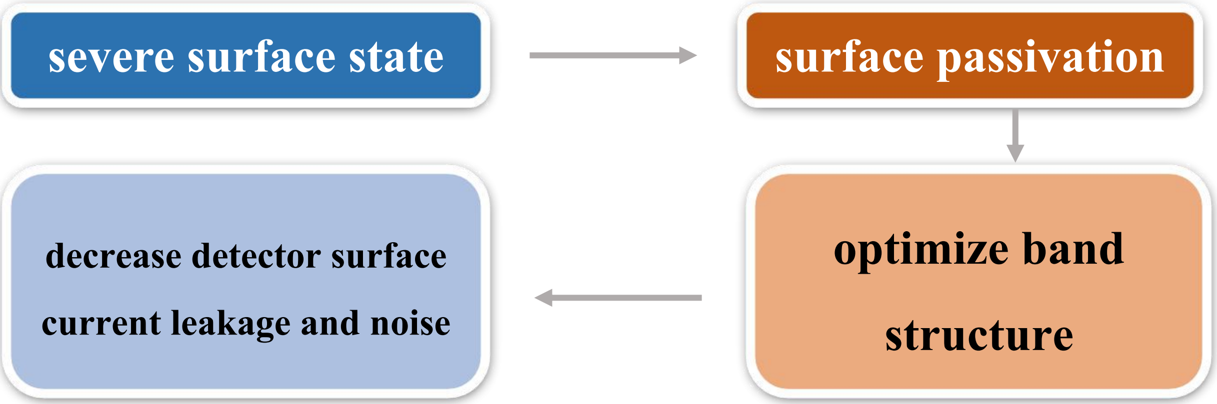
[1] 杨丽桃. 基于CDEX-1B点电极高纯锗探测器的暗物质直接探测[D]. 北京：清华大学，2017：25

[2] SZE S M. Semiconductor devices： physics and technology[M]. John wiley & sons，2008

Surface passivation

Protection layer

- ❖ Eliminate pollutants
- ❖ Eliminate surface dangling and stress bonds
- ❖ High resistance
- ❖ Blocking hole or electron carrier injection



HPGe detector is bare immersed in liquid nitrogen with long-term, and the leakage current could tend to increase.

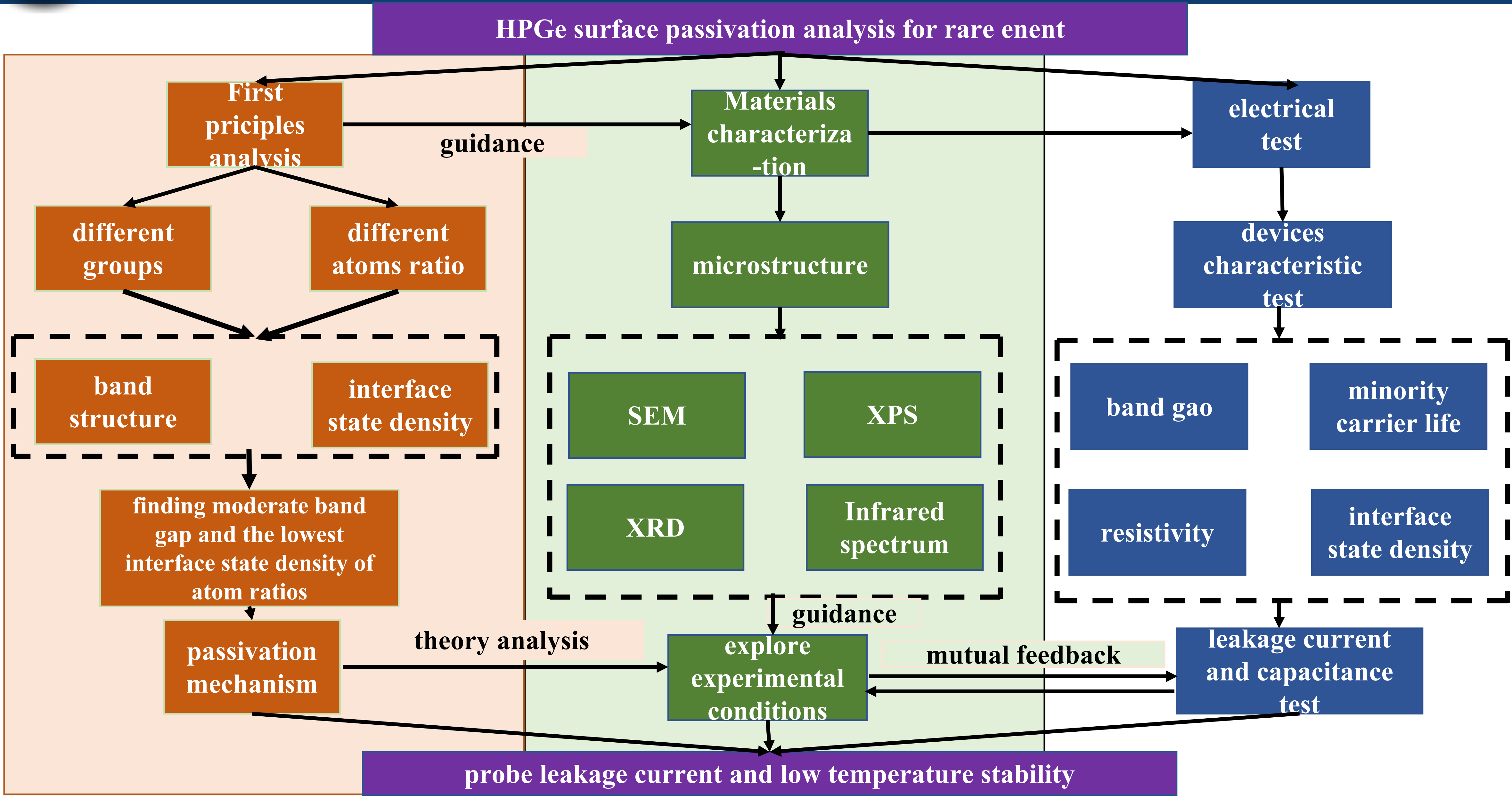
Solution: Passivation of HPGe detector

Achieve **low leakage current** and **low threshold of detector**

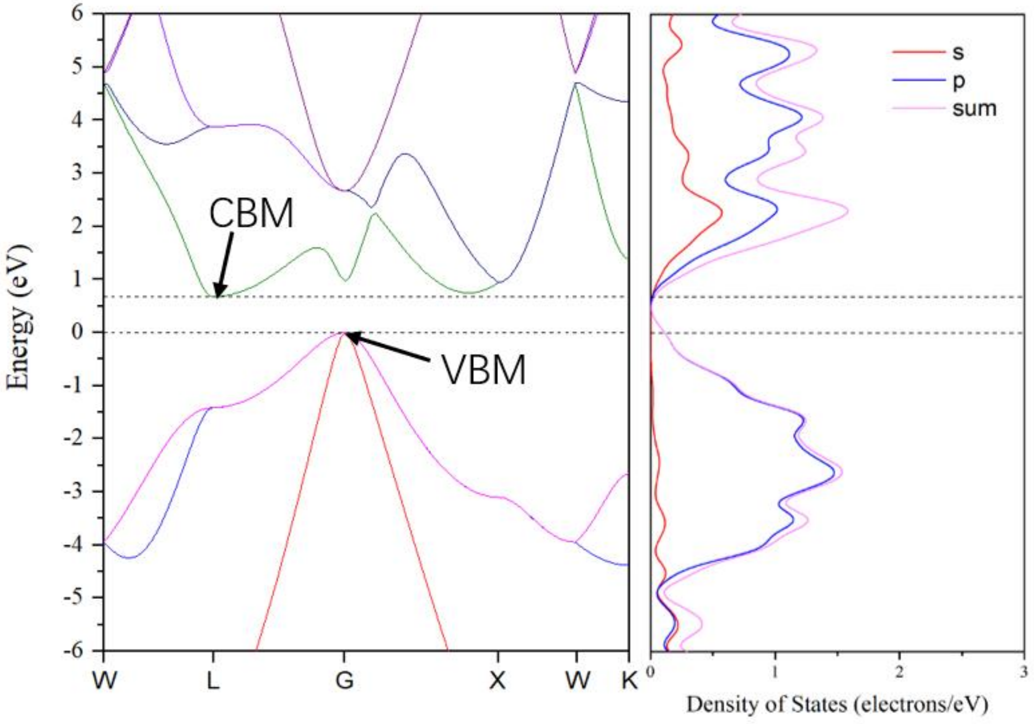
Realize stable operation of HPGe **barely immersed in liquid Nitrogen or Argon**

- **Background**
- **First-principle Simulation, Passivation Evaluation and Performance of HPGe detectors with Silicon oxide Films**
- **Prophase Simulation, Film Fabrication, Passivation Evaluation on Germanium Oxynitride passivation of Ge-based Devices**
- **Conclusion and Future Plan**

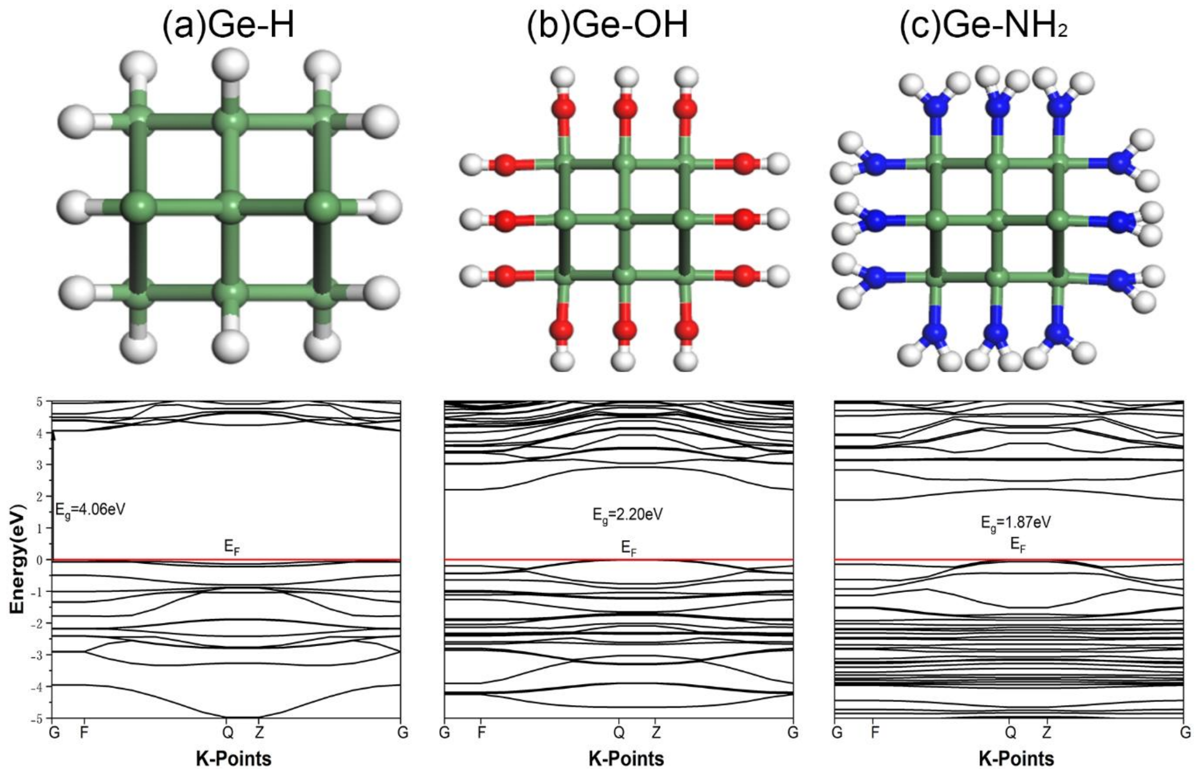
Methods


HPGe surface passivation analysis for rare enent
First principles analysis
guidance
Materials characteriza -tion
electrical test
different groups
different atoms ratio
microstructure
devices characteristic test
band structure
interface state density
SEM
XPS
XRD
Infrared spectrum
band gao
minority carrier life
resistivity
interface state density
finding moderate band gap and the lowest interface state density of atom ratios
guidance
passivation mechanism
theory analysis
explore experimental conditions
mutual feedback
leakage current and capacitance test
probe leakage current and low temperature stability

First-Principle Simulation



Band structure and DOS of Ge (100) direction



Cross section of –H, -NH_2, -OH passivation: (a) Ge-H, (b) Ge-NH_2 , (c) Ge-OH

Surface passivation changes the composition of conduction band and valence band edge electronic states to realize the regulation of band edge characteristics.

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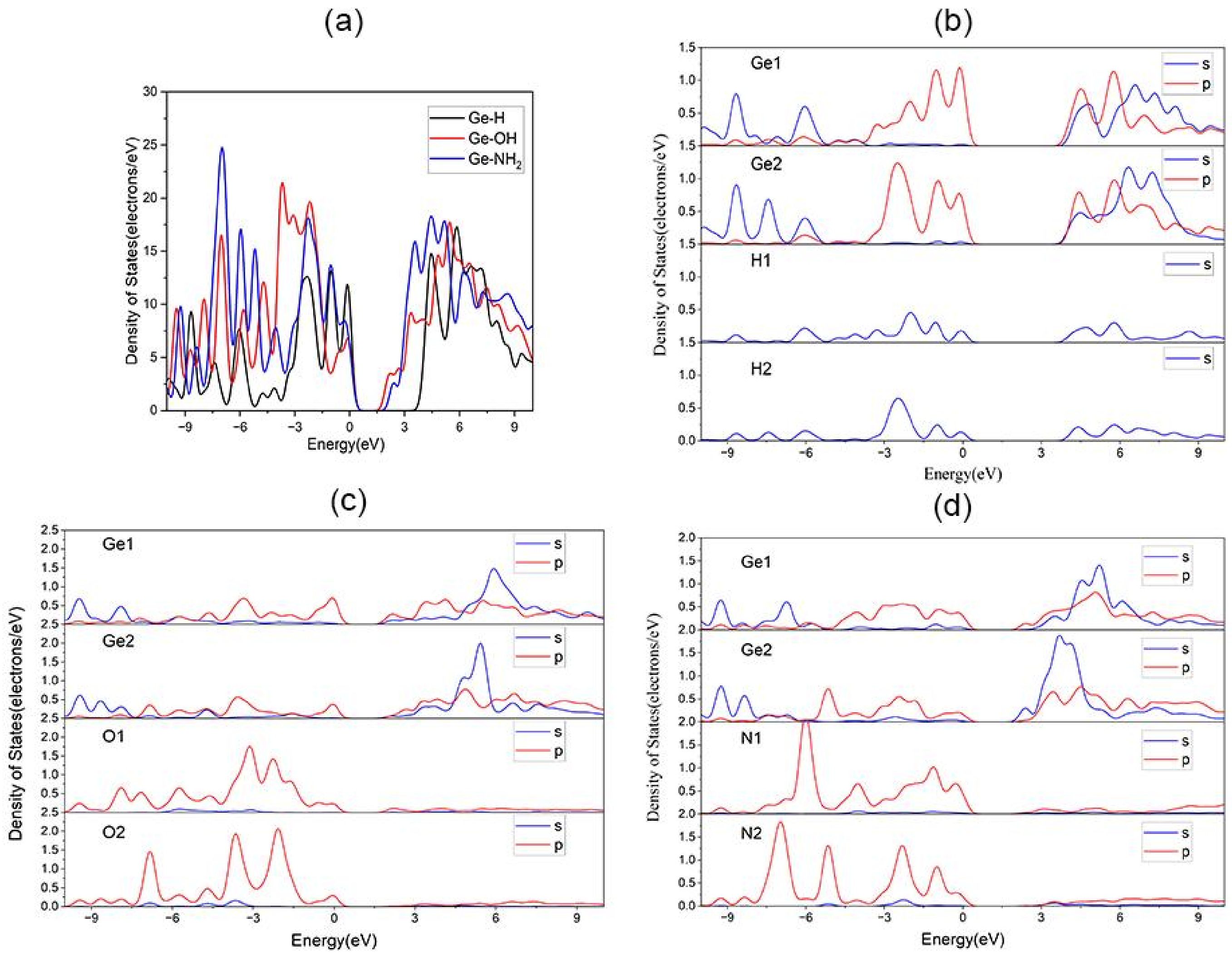
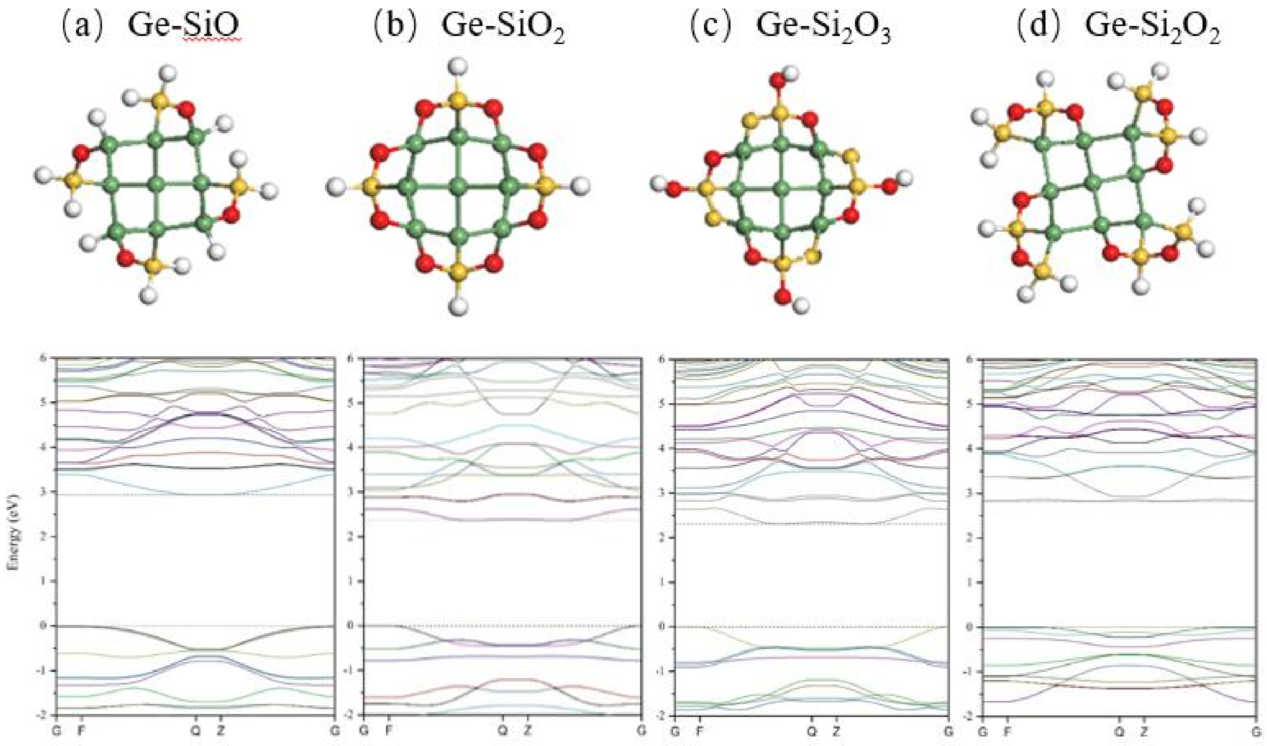
First-Principle Simulation



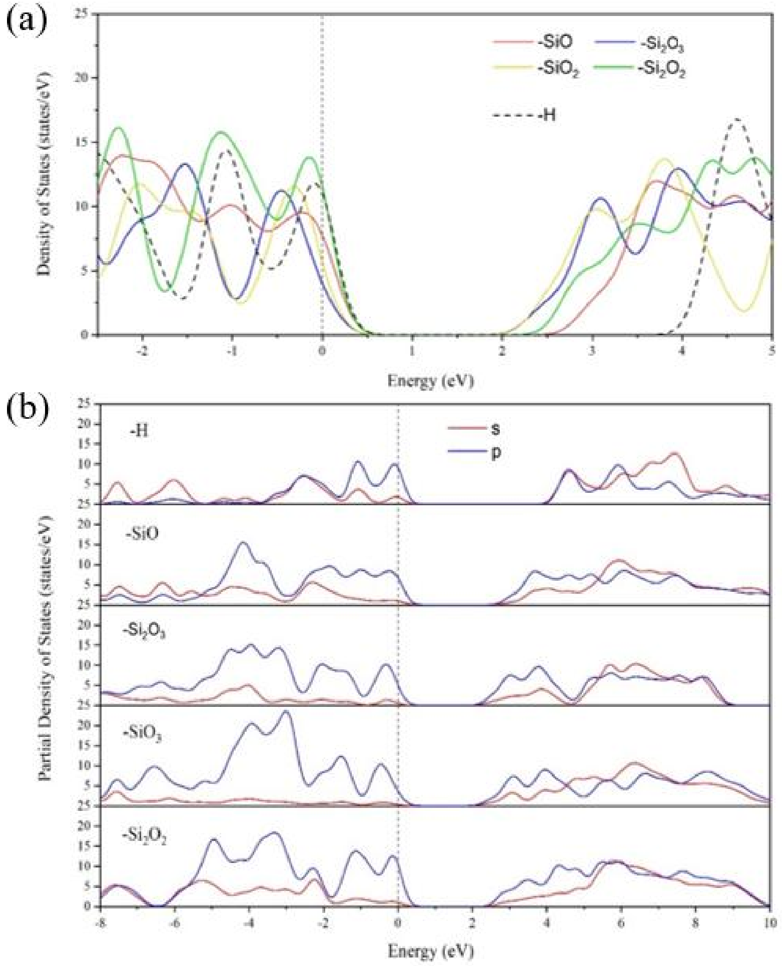
DOS of Ge-H，Ge-OH和Ge-NH_2 （a）TDOS；（b）-H PDOS；（c）-O PDOS；（d）-N PDOS

- **N passivation has a direct bandgap, while O passivation transforms into an indirect bandgap**
- **Ge-OH has the best passivation effect.**
- **The strong electronegativity of O and N results in the rearrangement of electron cloud and the change of electron state distribution at the band edge.**
- **Passivation of -O and -N leads to increased surface recombination efficiency and surface leakage current, which affects surface charge collection.**

SiOx Passivation by First-Principle Simulation



Cross Section and Band structure of SiOx: (a) -SiO，(b) -SiO_2， (c) -Si_2O_3， (d) -Si_2O_2

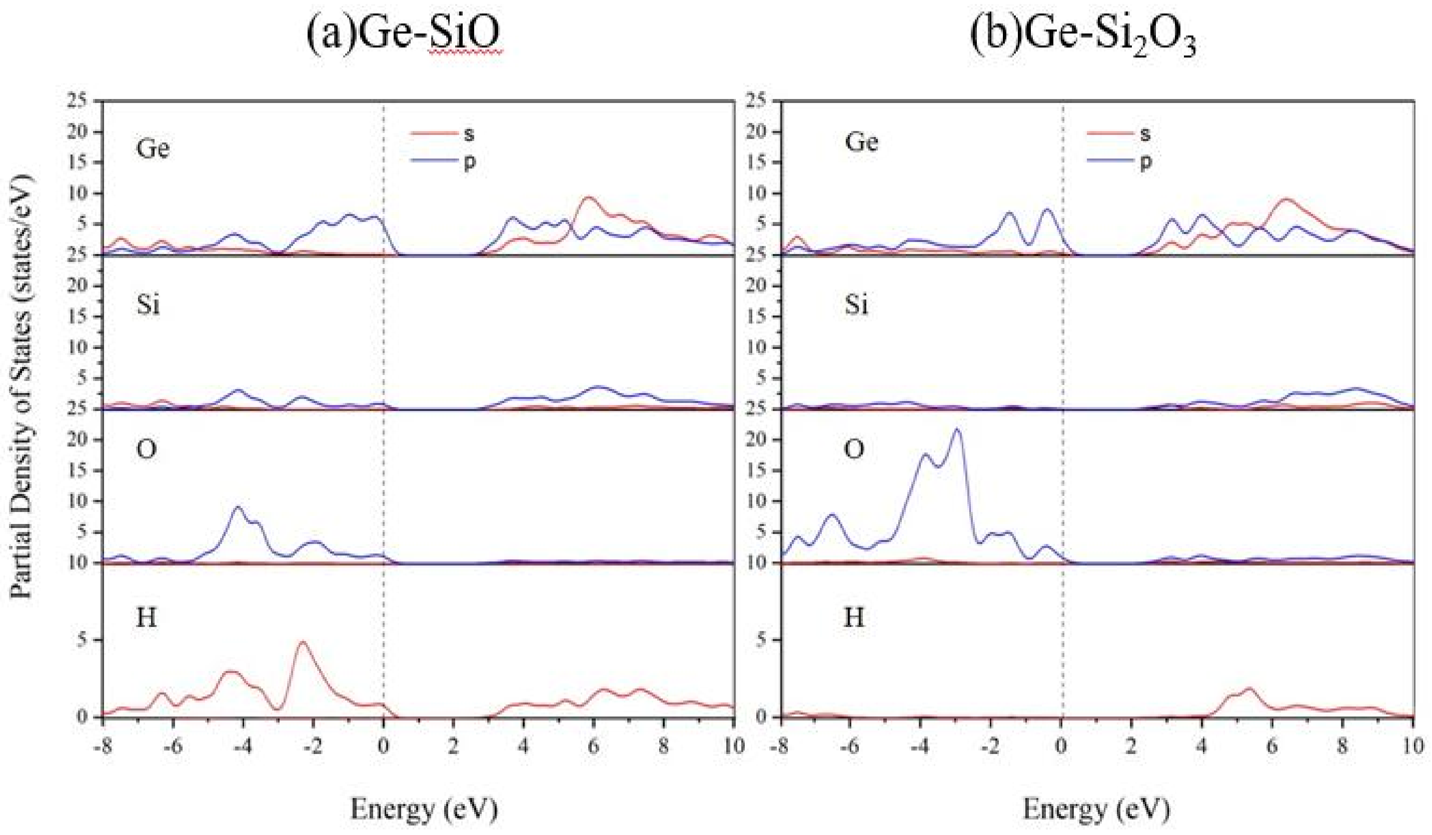


SiOx DOS: (a) TDOS, (b) Partial Density of State

Band structure: indirect band gap, lower band gap width than H passivation

Shasha Lv, et al. Nuclear Science and Techniques (2021) 32:93.

SiOx Passivation by First-Principle Simulation

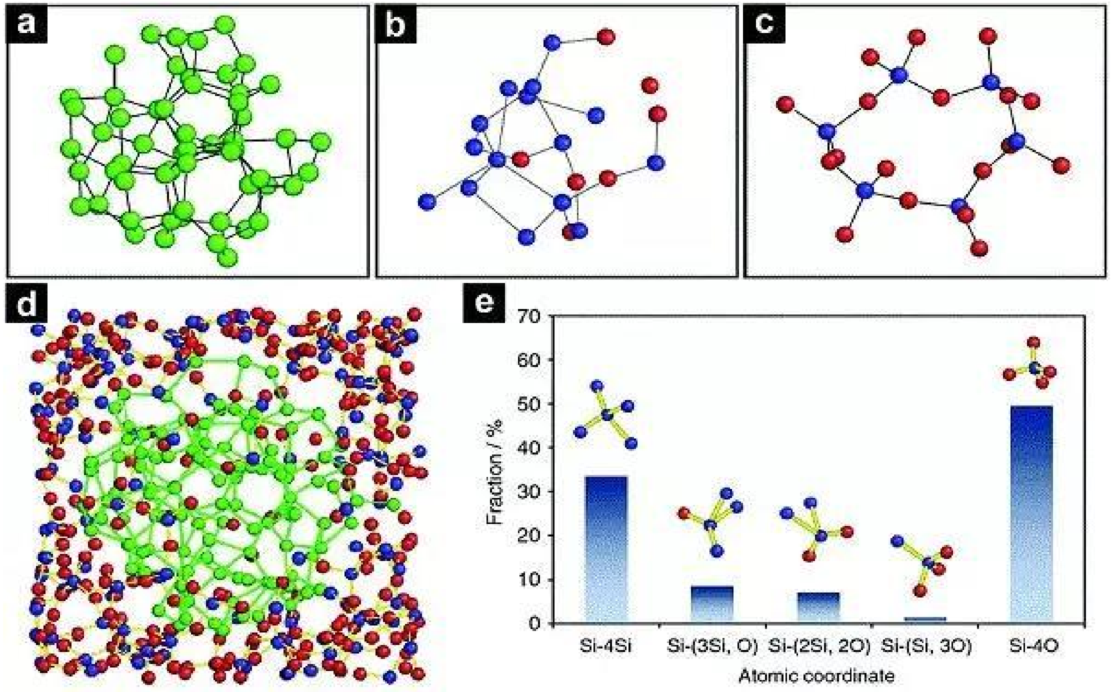


Ge-SiO and Ge-Si_2O_3 Partial Density of State: (a) Ge-SiO, (b) Ge-Si_2O_3

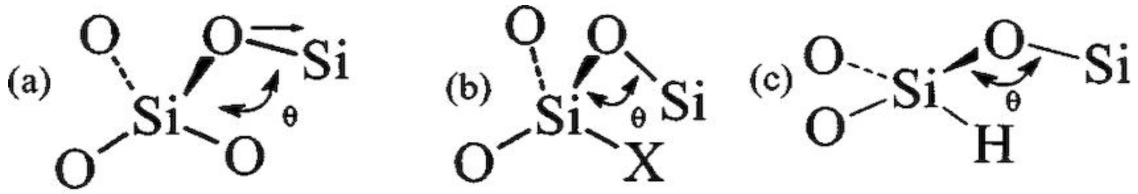
- **The density of states of different silicon oxygen atoms passivated significantly decreases compared to H passivation.**
- **The SiOx system reduces the DOS intensity and interfacial state density, and the fixed charge in the oxide layer forms an internal electric field.**
- **The passivation effect of Ge-SiOx is better with increase of O element.**
- **Si/O atoms are randomly mixed/bonded in Ge passivation layers with excellent electrical and chemical passivation properties**

Shasha Lv, et al. Nuclear Science and Techniques (2021) 32:93.

SiOx Film by Electron Beam Evaporation



Flexibility of SiOx

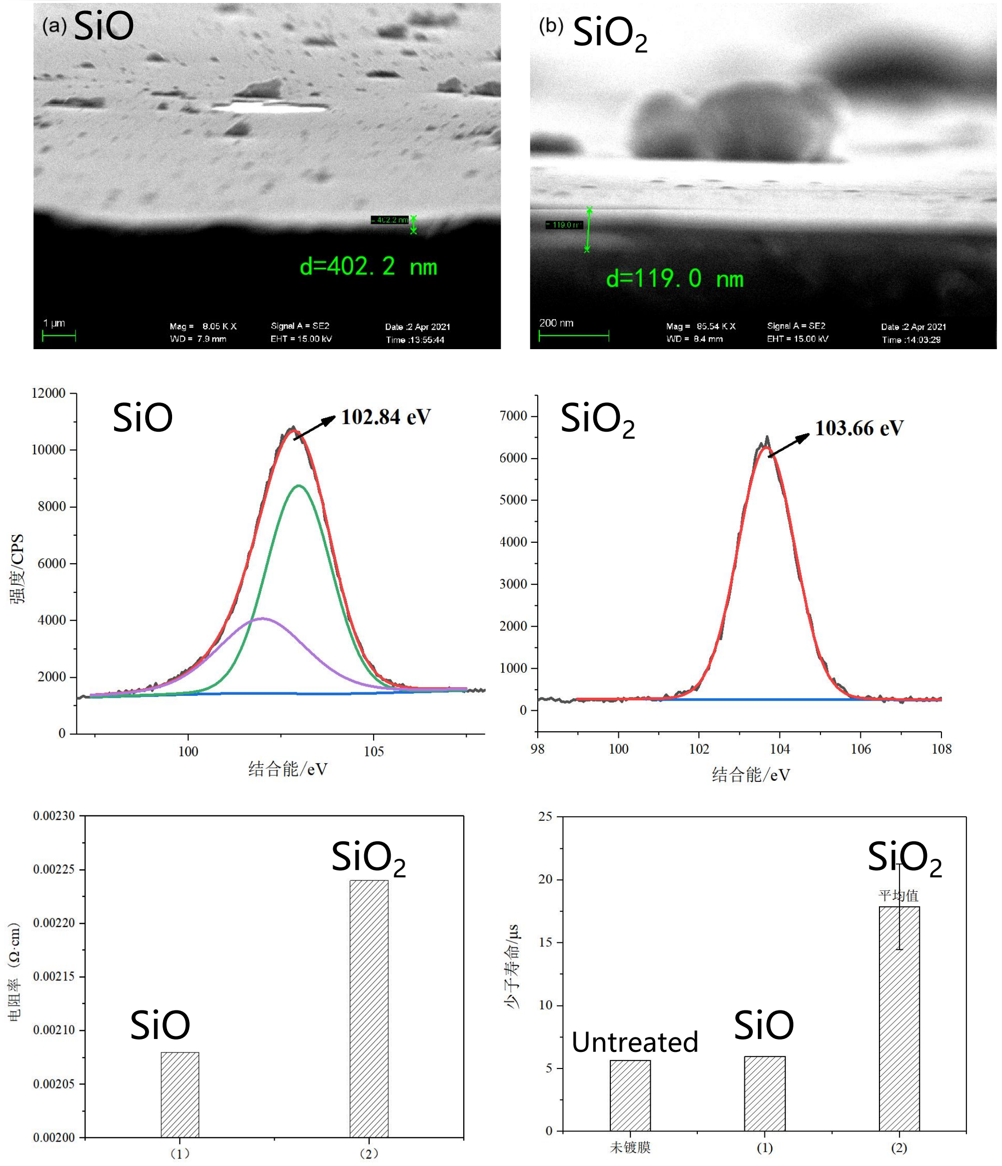


- SiO (SiOx) : Microstructure is controversial: random bonding model, random mixing model, interfacial cluster mixing model.

- SiO_2: The flexibility of Si-O-Si bond makes SiO_2 have a variety of crystal forms and makes most of the chemical bonds at the interface remain saturated; There is a large amount of fixed positive charge in SiO2, which can produce field effect passivation.

A. Hirata, et al, Nat. Commun., 2016, 7, 11591

SiOx Film by Electron Beam Evaporation



SEM, XPS and Minority lifetime analysis

表1 不同靶材样品XPS分析数据

样品编号	靶材	Si峰中心位置	Si峰面积	O峰面积	Si：O
①	SiO	102.74	25454.1	132319.5	1:1.40
②	SiO_2	103.66	14109.0	103095.7	1:1.97

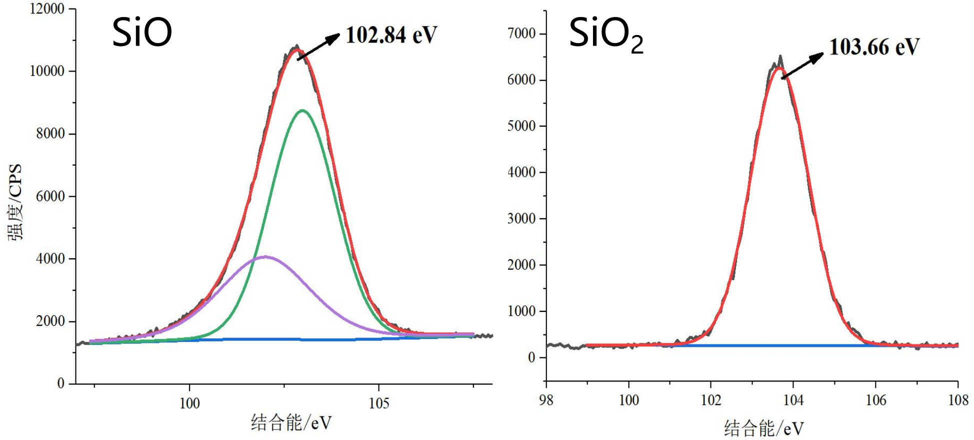


图3 不同靶材样品XPS能谱图

SiOx Film by Electron Beam Evaporation

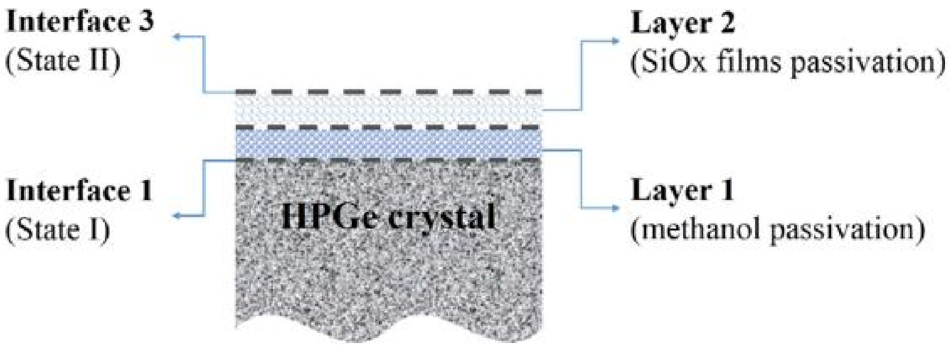
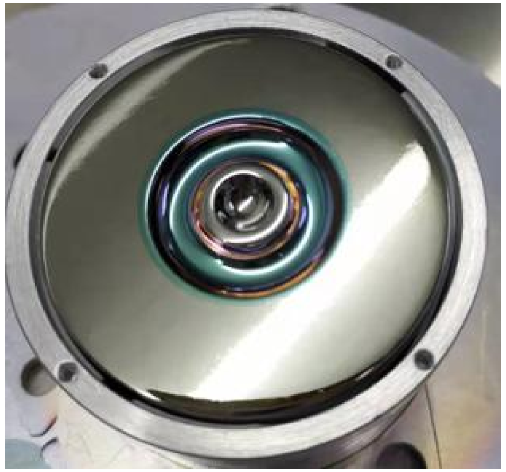
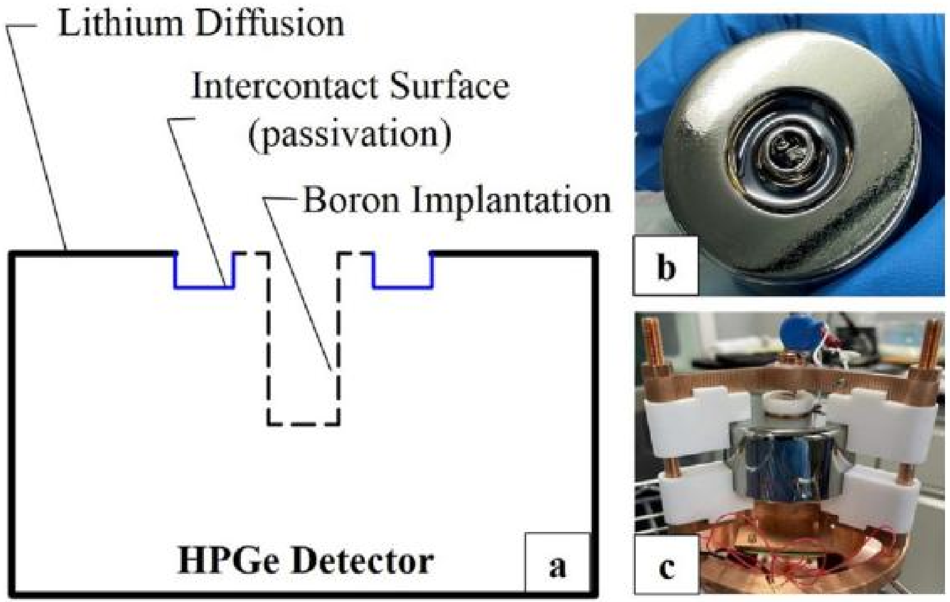


Fig. 1. Schematic diagram of surface passivation of a HPGe crystal.

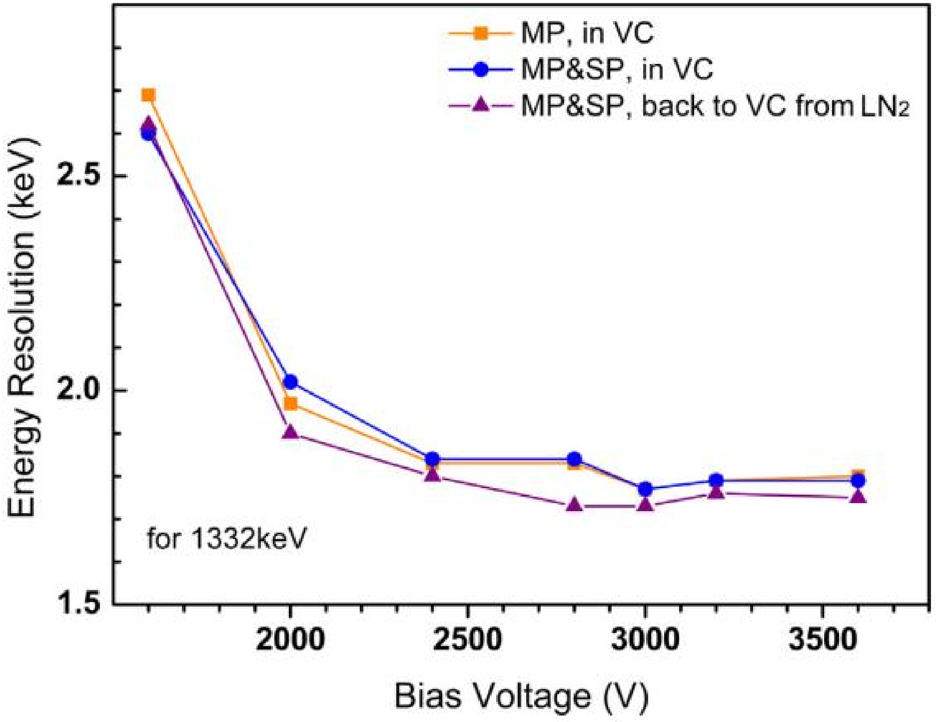




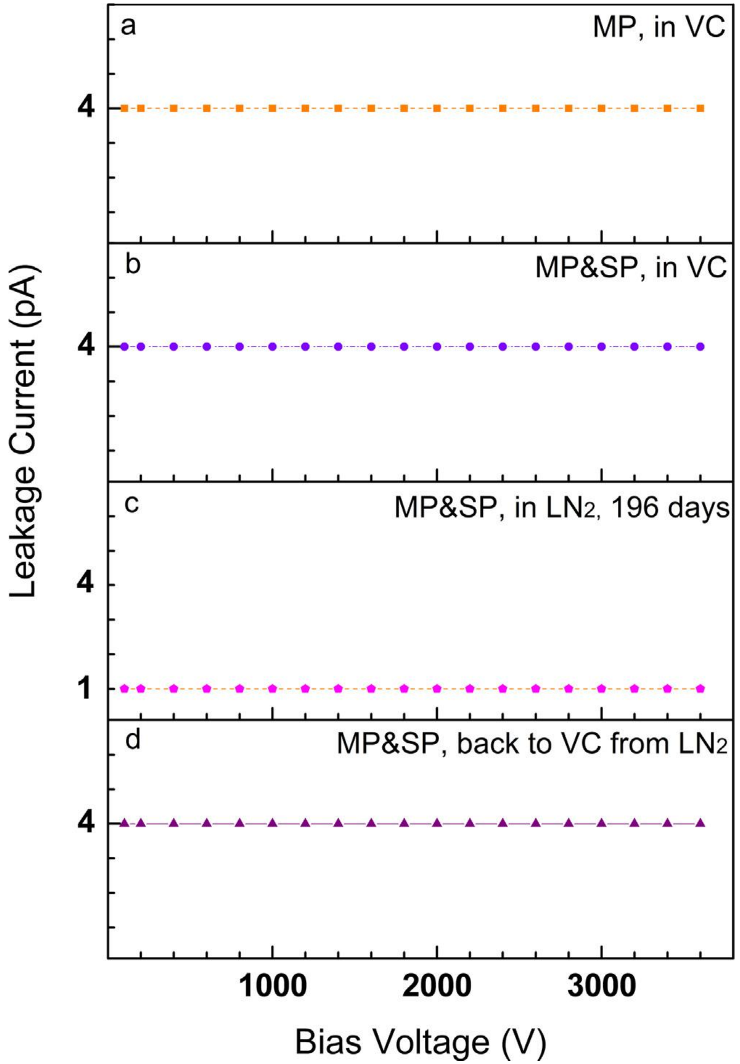
Two steps passivated HPGe

Methanol passivation, SiOx films passivation, bare immersion in LN2

SiOx Film by Electron Beam Evaporation



Resolution of the detector (FWHM) as a function of the bias voltage at different stages



Leakage current was monitored at all the critical process stages

液氮裸泡探测器性能：
能量分辨率：FWHM范围1.80至1.5 keV
液氮环境中工作196天，在工作电压3600 V，耗尽电压1800 V下，维持超低漏电流（1 pA）

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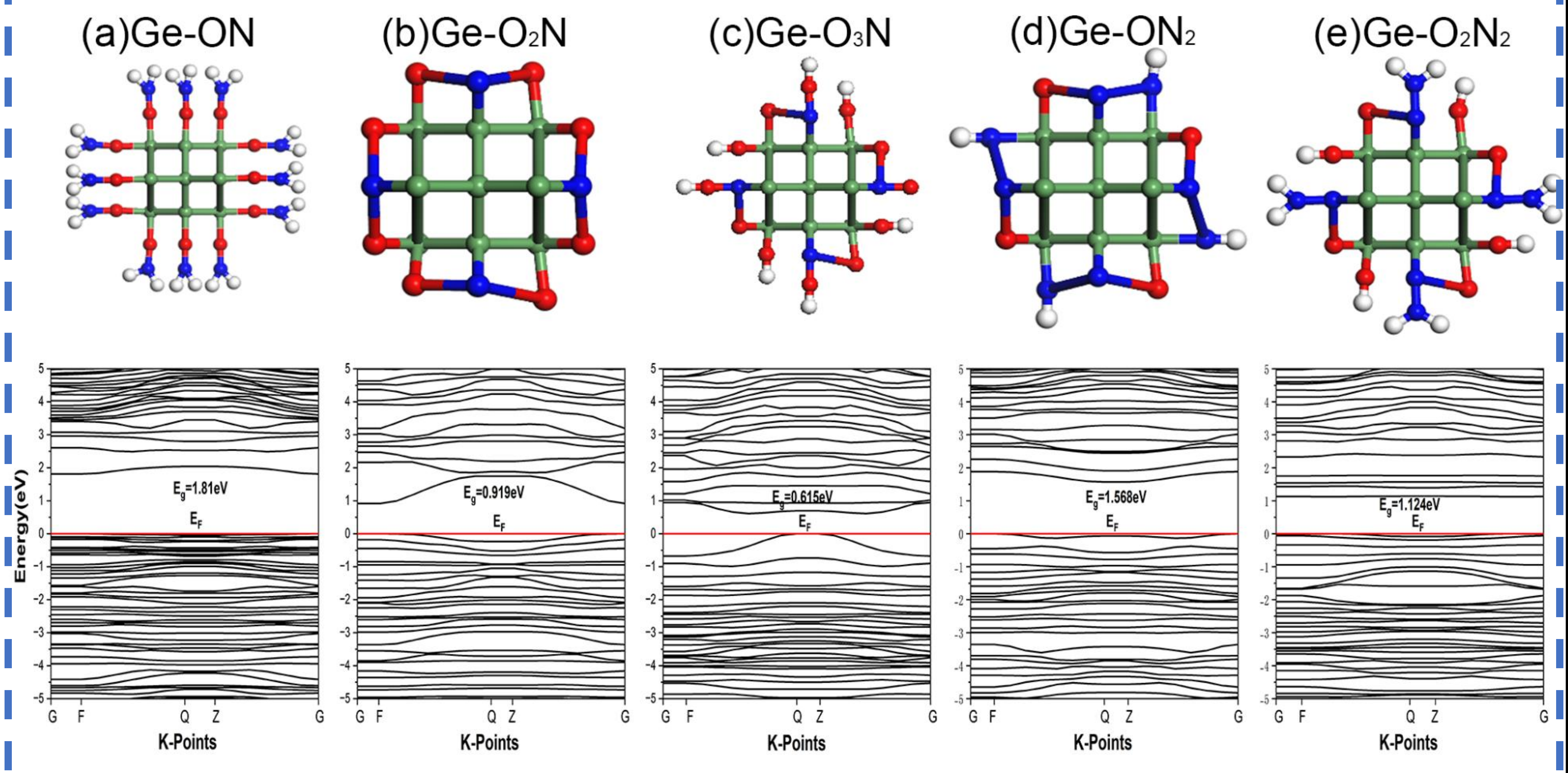
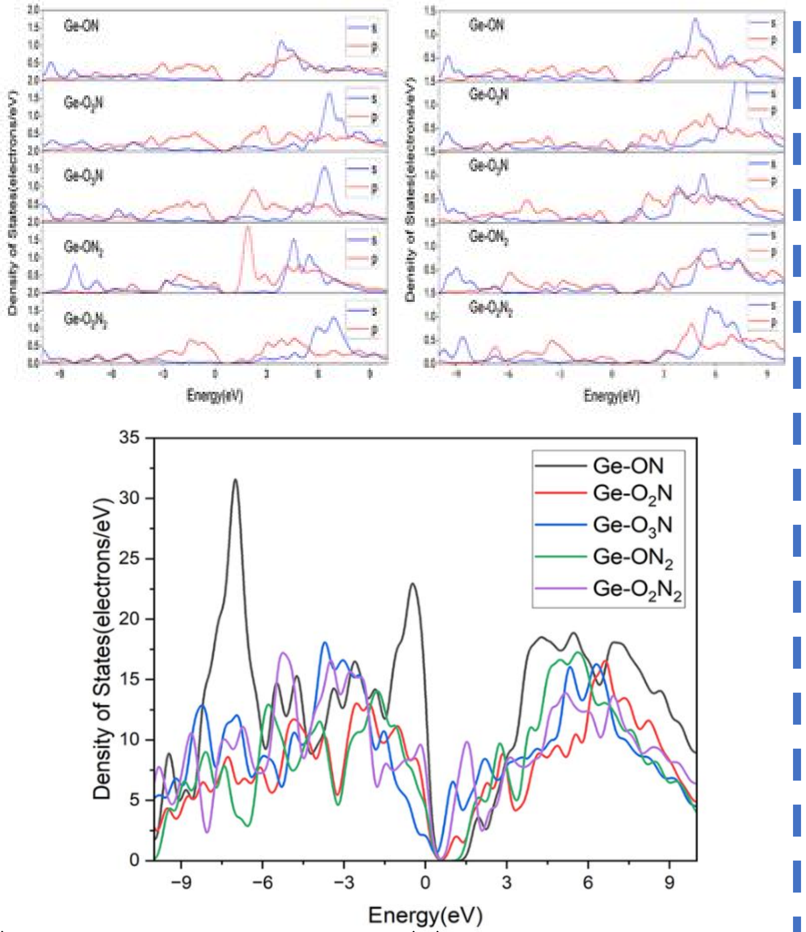
GeOxNy by First-Principle Simulation



Five different N_2:O_2 ratios of germanium oxynitride: （a）-ON； （b） O_2N； （c） O_3N； （d） ON_2； （e） O_2N_2

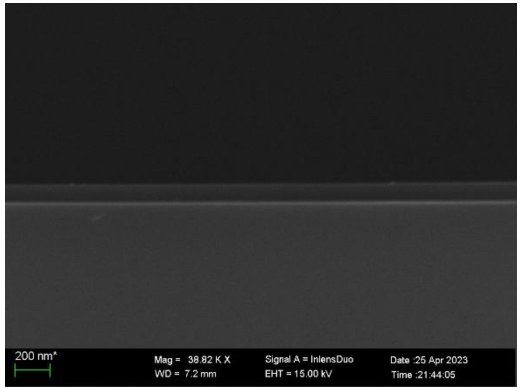


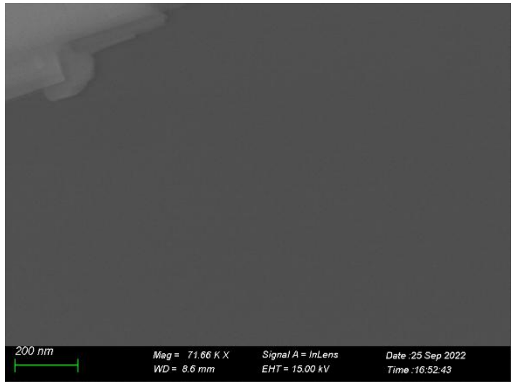
（a）PDOS of one dangling bond； （b）PDOS of two dangling bond； （c）TDOS of five different ratios of germanium oxynitride

DOS of -O_3N is the lowest but not the optimal choice

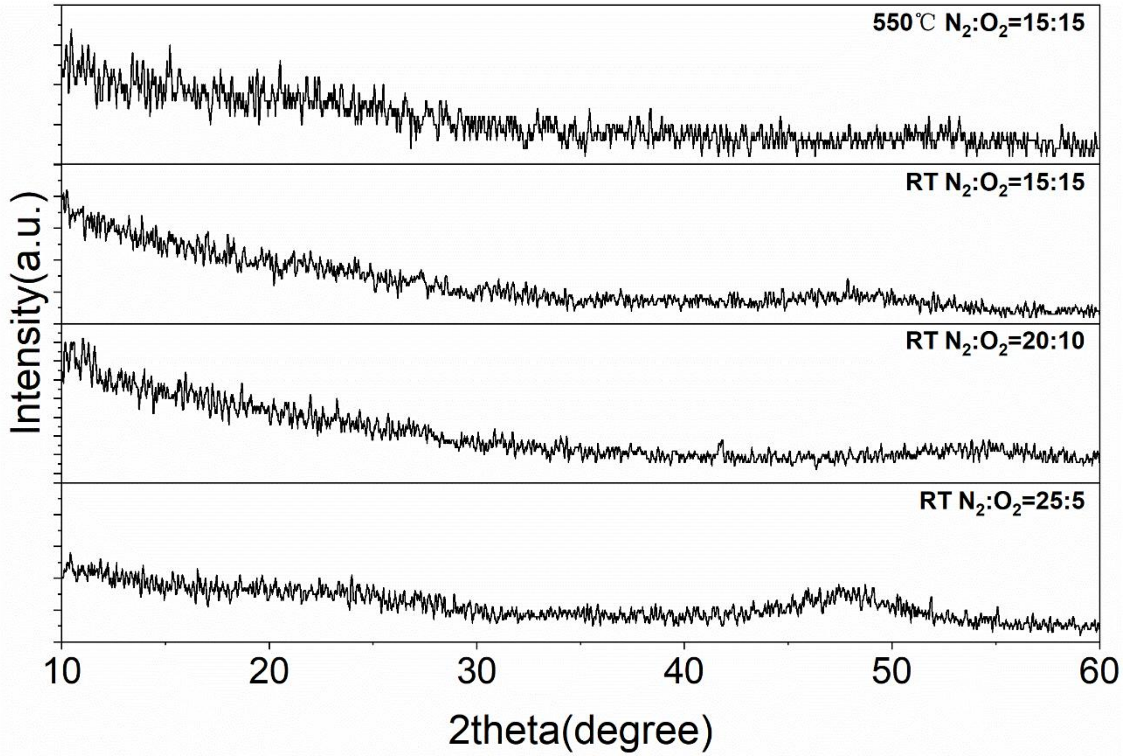
DOS -ON_2 is the best, which the lower DOS and moderate band gap

GeOxNy Film Preparation

（a） 

（b） 

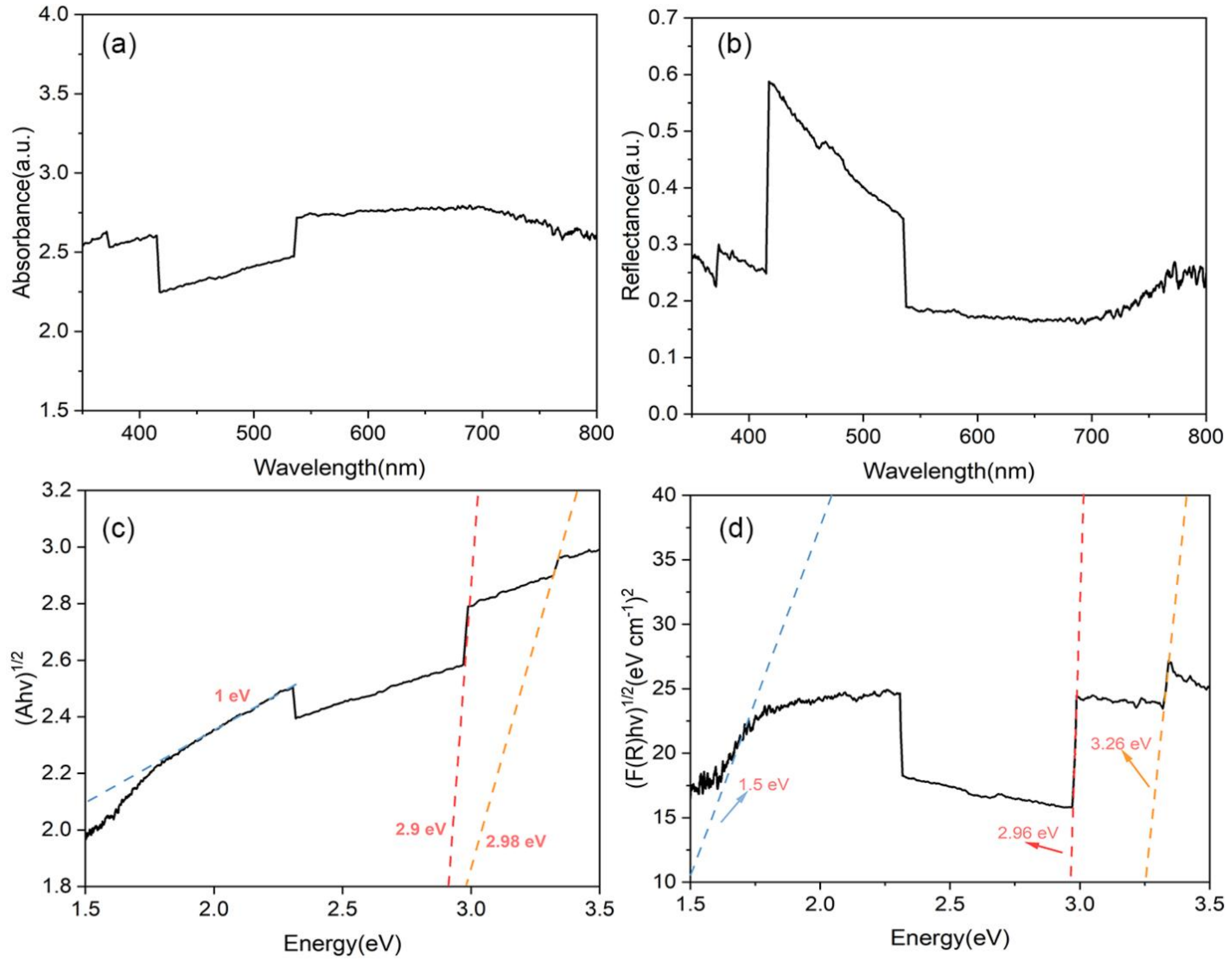
Nitrogen and Oxygen as sputtering atmosphere oSEM（a） passivation cross section；（b）Surface morphology



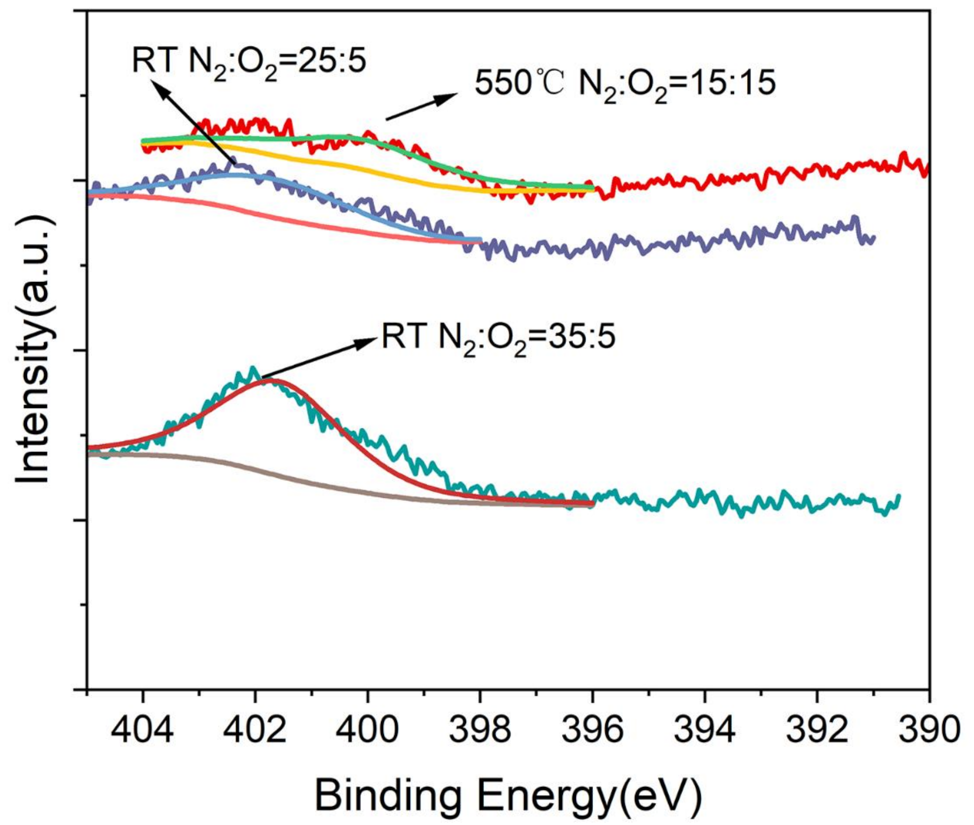
XRD spectrum of different N_2 O_2 ratio

- **Homogeneous film**
- **The amorphous state is strong and the growth is reverse random**

GeOxNy Film Preparation



(e) UV-vis absorption spectrum; (f) Tauc plot fitted band gap;
(g) UV-vis reflection spectrum; (h) Tauc plot fitted band gap

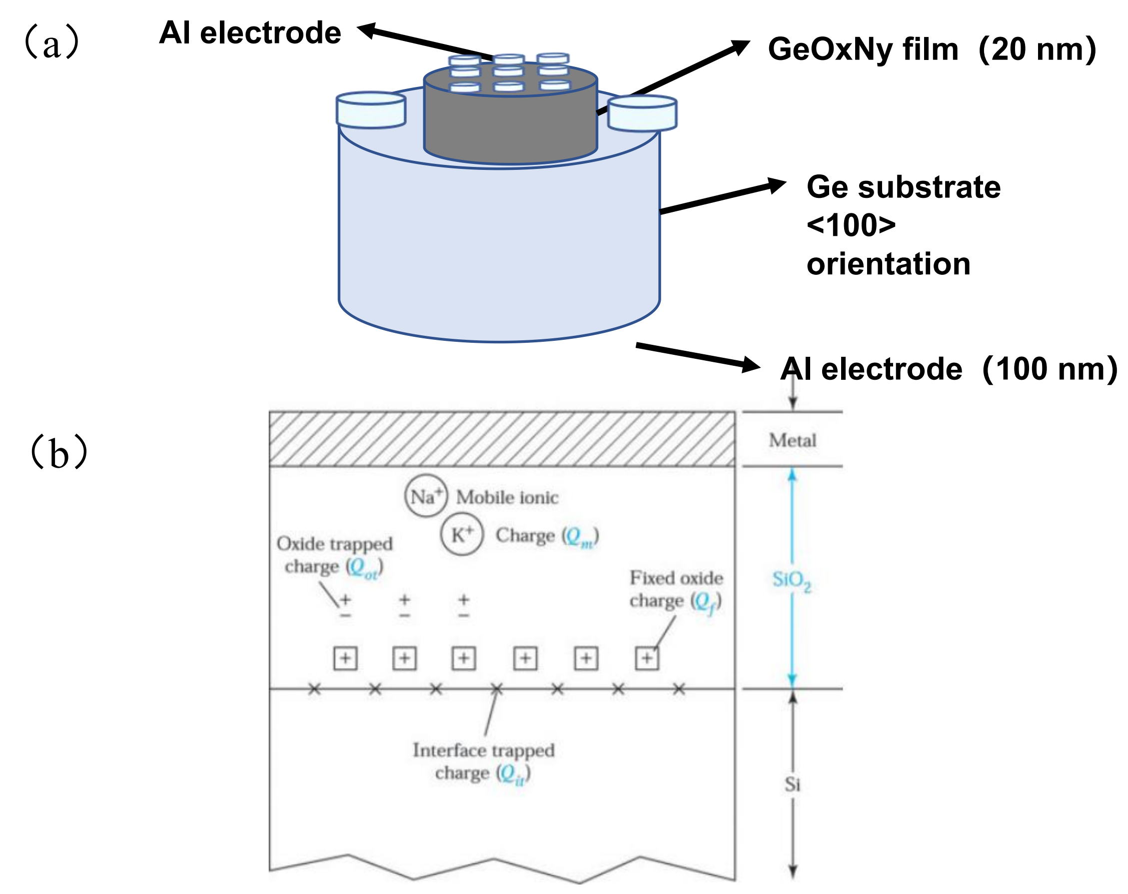


N1s energy level XPS spectrum

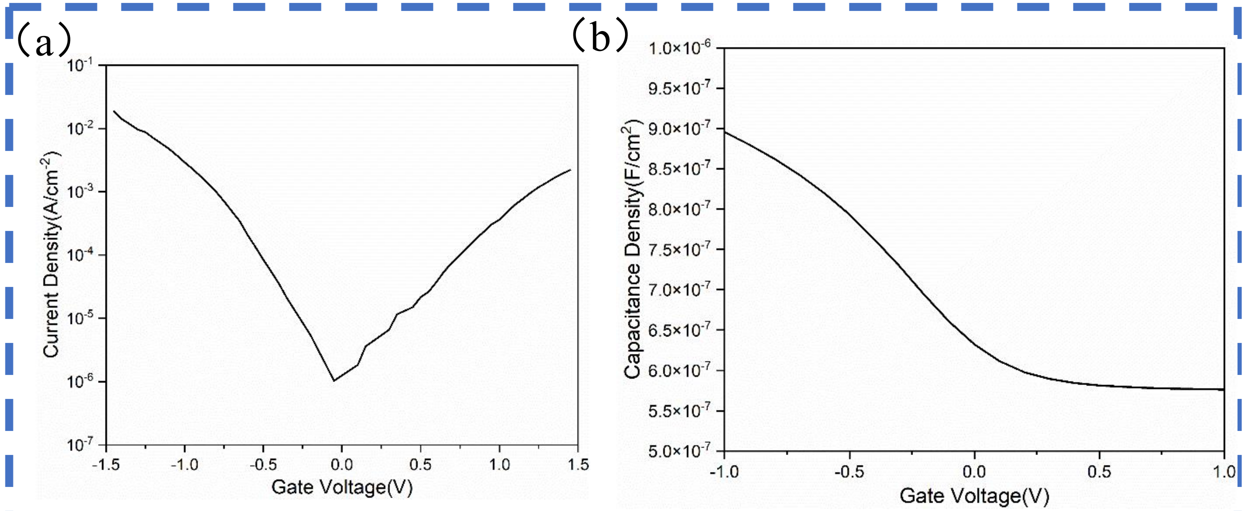
- Less O_2 get GeO;
- Too much nitrogen will prevent the formation of germanium nitride.

GeOxNy Passivation Evaluation

GeOxNy/Ge interface defect analyze



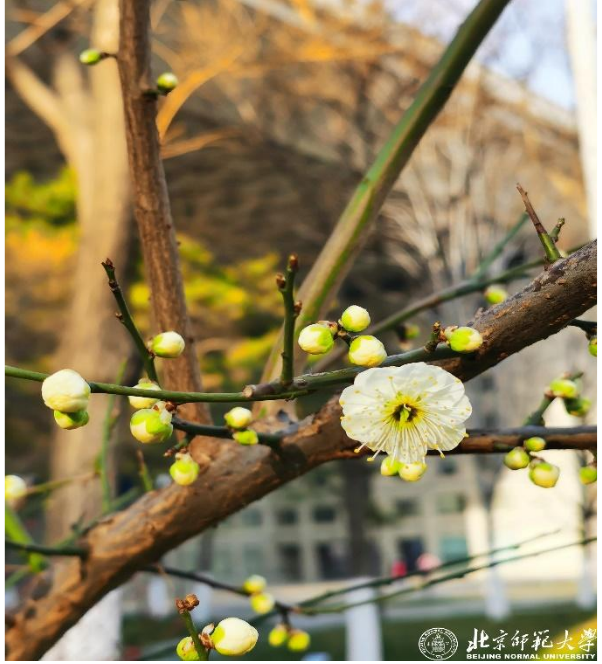
（a）GeOxNy MOS capacitance diagram；（b）MOS oxide layer influence factor[1]



GeOxNy passivation layer electrical character（a）I-V character；（b）C-V character

- **The passivation layer is mainly affected by interface trap charge.**
- **Flat band voltage is about -0.8V;**
- **Passivation layer thickness is thin, easy to be broken down**

[1] SZE S M. Semiconductor devices： physics and technology[M]. John wiley & sons，2008



Thanks for your listening

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