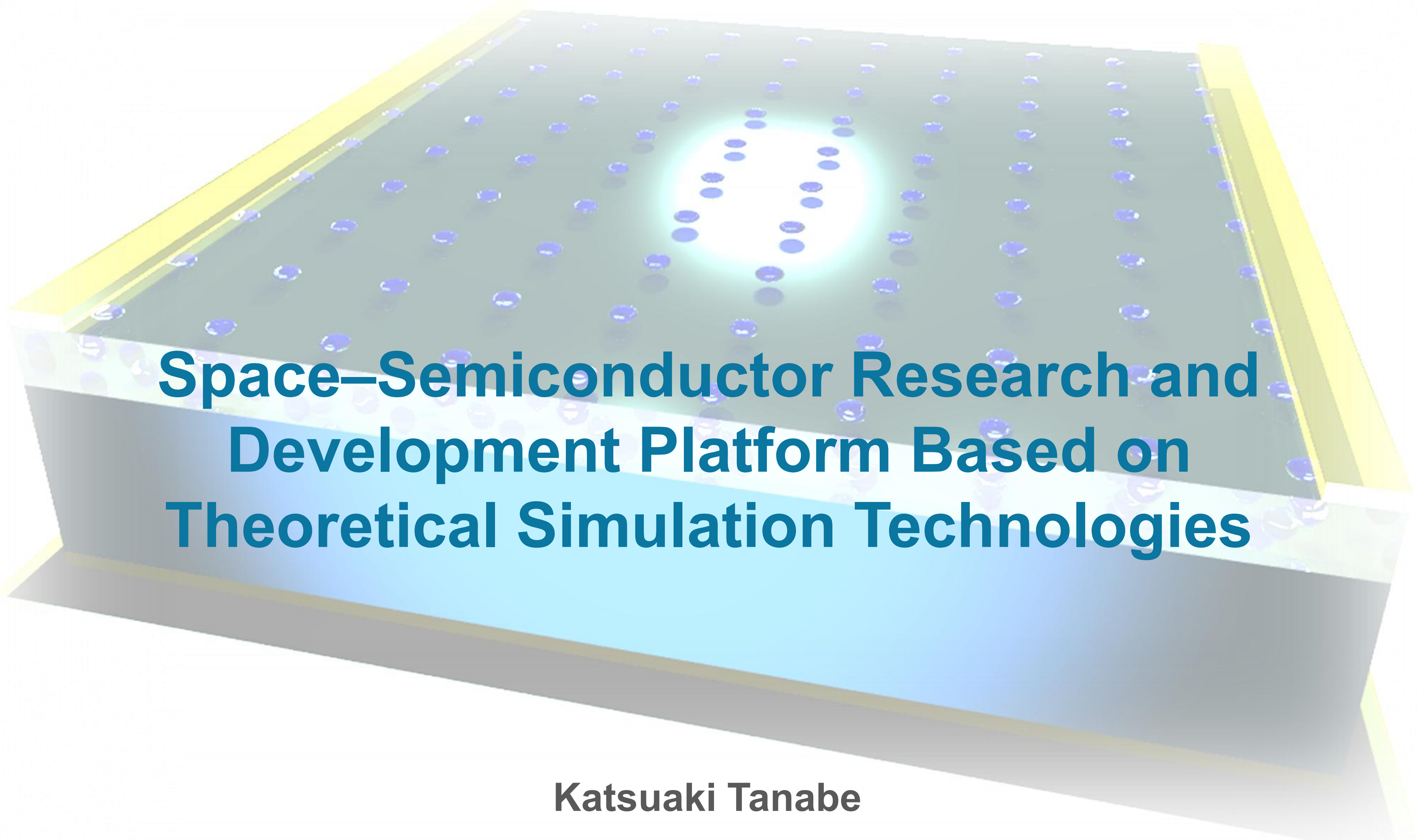

Space–Semiconductor Research and Development Platform Based on Theoretical Simulation Technologies

Katsuaki Tanabe

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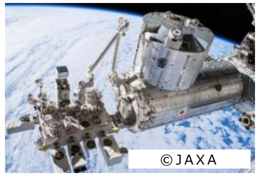
Overall Contents of the Project

Development of Space Environmental Simulations for Next-Gen Semiconductor Industries

Users' Requirements

Space env. use ⇔ R&D costs

Understanding of complex phenomena | **Continuous in-orbit experiments**



Current Technical Issues

- Parallel processes and strong correlation among **G-L-S phases**
- Handling difficulty of time & space **scale discrepancies** > six digits
- **Insufficient expt. data** in micro-gravity, plasma/irradiation env.
- Requirement of coupling schemes for **incompatible phys. models**

Material
Materials design ·Crystal quality

Process
Growth·Etching ·Surface chem.

Device
Assembly·Pack-aging·Reliability

- **Various computational schemes** (eg, MD, CFD, DFT, heat transfer, TCAD) need to be combined, but each has its own **application range and limitations**

Project Contents

(Space)

Space environment simulations for space experiments

Feedback from space expt. results for simulation accuracy

μ-gravity | Irradiation | Severe *T* | High vac.

Space env. simulation platform

Solid·Liquid·Gas | Time·Space scales | Properties | Calc. methods

Enabling complex large-scale calc. across materials, processes & devices

Use of understood mechanisms in on-ground manufacturing to improve products, efficiency & costs

(Ground)

Connecting univ., res. inst. & corp. across Japan from Kyoto

Collaborative hub

Space–ground co-enforcement

Overcoming structural defects

Community | Collaboration | Value seeds

Edu-cation | Funds

Contrib. to Semicon. Ind.

Space env. use
- ✓ Predicting space expt. results
- ✓ Providing challengers' env.
- ✓ Reducing barriers

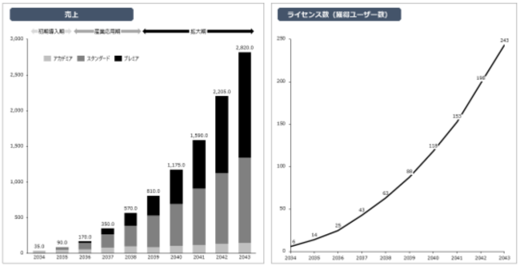
Industry use
- ✓ Issue solution
- ✓ Generalized, open knowledge for improving functions

Collaboration
- ✓ Res. tool infrastructure for whole industry
- ✓ Ind.–Gov.–Acad. platform

HRD·exchange
- ✓ Fostering tool for next-gen researchers open to stundents & younger workers

Markets to be generated

- Widely accessible **cloud service** with flexible plans for res. inst. & corporations
- 350M JPY in 1st yr, to be expanded to **2.8B JPY in 10 yrs**
- **Int'l defact standardization** by targeting global clients



Background of the Project : User Needs

In the semiconductor field, many unresolved phenomena can be elucidated only in the space environment—such as microgravity, vacuum, and radiation—and reproducing and understanding these phenomena has become a critical challenge for industry. However, space experiments are expensive, time-consuming, and difficult to conduct multiple times, making it hard for companies to engage in sustained efforts and resulting in a structural barrier to advancing space-based R&D. This gap—“high necessity but difficult to execute”—is the starting point of this project.

R&D needs for elucidating “unresolved phenomena” using the space environment

A large number of semiconductor elemental technologies involve phenomena that can only be understood in space.

- Microgravity : Understanding crystal growth mechanisms in the absence of convection
- Vacuum, low temperature, and high temperature : Understanding material interfaces and phase transitions
- Cosmic rays : Elucidating defect generation and degradation mechanisms

Stagnation of corporate participation caused by the high-cost structure of space expt.

Space experiments are expensive and time-consuming, creating a “one-shot” structure that becomes a barrier to entry.

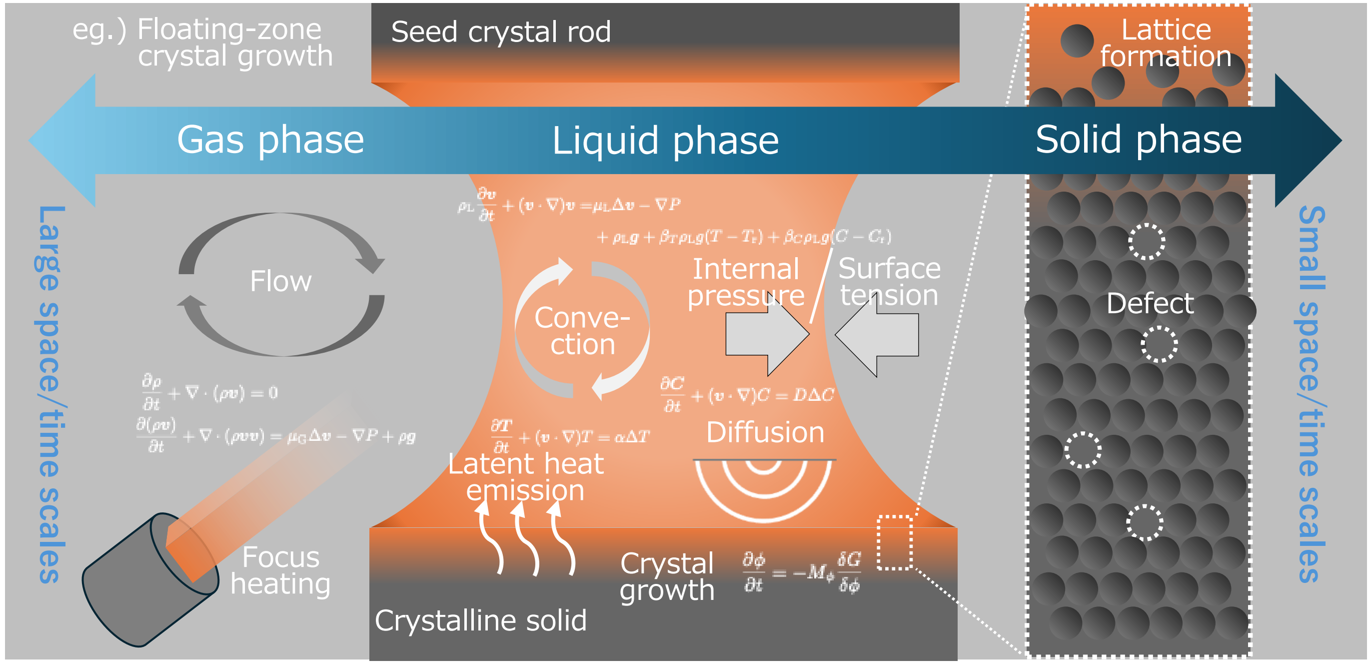
- Experiment costs range from tens of millions to several hundred million yen per attempt
- Lead times of six months to several years from preparation to sample recovery
- Although iterative experiments are essential for optimization, securing budgets for multiple rounds is extremely difficult

Background of the Project：Technological Issues

Conventionally manufacturers have relied on empirical optimization because the complex phenomenal mechanisms are not well understood. Moreover, the space environment has further complexities, such as microgravity, radiation, severe temperatures, and extreme vacuum, all of which we have to handle!

Issues in Semiconductor Manufacturing

- **Complexity in multi-phase coupling :**
  Various models required to reproduce correlated multiphases
- **Discrepancy in the space/time scales :**
  Over six-digit gap in each, hindering direct whole simulations
- **Insufficiency in phys. props & conditional dependencies**
- **Incompatibility in mathematical models :**
  High-level coupling required to unify multiple processes



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Issues Specific to the Space

Cosmic radiation damage	Difficulty in reliab. eval. by insufficient expt. data for high-energy particle damages
Thermal management	Heat release from devices in vacuum insulation & absence of convective transport
Convection & growth in m-grav.	Prediction difficulty for melt growth, defect formation etc. by anomalies of Marangoni conv. in μ-grav.
Unexplained melt growth mechanism	Uncertainty in space env. by sim-expt discrepancy in the lack of fundamental S–L interfacial mechanism understanding
Degrad. prediction, multiscale analysis	Unestablished multiscale analysis across defect formation and degradation for long-term reliability prediction
Irradiation expt. eval. & modeling	Insufficient data of multi-effect eval. due to the limitation in ground reproduction of effects of γ-rays, neutrons, etc.
Complexity in lithography process	Application limitations of ground simulators by the physical changes in processes such as coating, development, etc. by μ-grav.
Next-gen materials & devices	Unestablished degradation mechanism, threshold control, etc. required for space reliab. of emerging SiC/organic semicond.

The Team

Principal investigator:

Katsuaki Tanabe, Kyoto University (Si, III–V, numerical simulations, AI)

Core members:

Kozo Fujiwara, Tohoku University (Crystal growth, Si, other advanced materials)

Manabu Togawa, KEK (Irradiation physics, simulations, facilities)

Masahiro Nomura, University of Tokyo (Advanced heat dissipation principles)

Kenji Yoshimoto, Kanazawa University (Semiconductor processes, digital twins)

Takahiro Kawamura, Mie University (First-principle calculations, crystal growth)

Tsunenobu Kimoto, Kyoto University (SiC materials and devices)

Tatsuya Hinoki, Kyoto University (Irradiation effects in solid-state materials)

Souta Miyamoto, Kyoto University (Molecular dynamics simulations, AI)

Chihaya Adachi, Kyushu University (Organic semiconductor materials and devices)

Supporting members:

Yusuke Mori, Osaka University (Nitride semiconductors, crystal growth)

Yoshihiro Kangawa, Kyushu University (Crystal growth simulations, informatics)

Several corporations from semiconductor and space industries

Project's Objective：Space Env.-Modeling Simulation Platform Dev.

Integrated simulation technologies that model and reproduce, across multiple scales, the behaviors of materials, processes, and devices arising under space-specific environments such as microgravity, radiation, and *T* fluctuations. -> A cloud-based platform capable of handling through crystal growth to device operation by linking the simulations with space expt. data, thus establishing a “common infrastructure” for space-based R&D.

01 Elucidation & modeling of materials

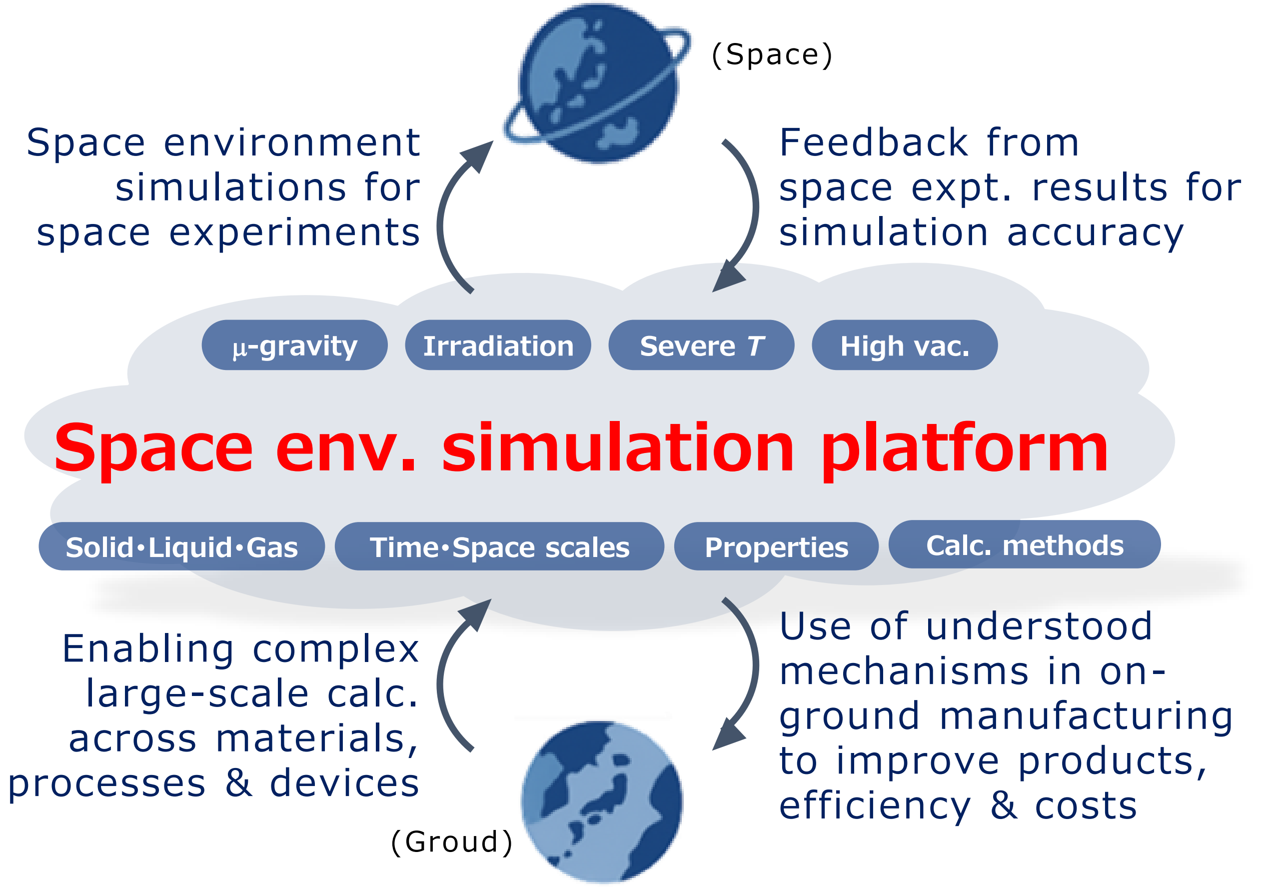
- Crystal growth mechanisms under microgravity (convection, interfacial behavior, defect formation)
- Modeling of dynamic phenomena at melt/solid–liquid interfaces for materials such as Si and AlN
- Multiscale analysis of defect generation, diffusion, and degradation induced by cosmic-ray irradiation

02 Modeling of processes in space env.

- Fluid and heat transport (CFD), chemical-solution processes, cleaning, and electroplating under μ-gravity
- Digital twin of lithography processes adapted for space environments

03 Long-term reliability & operational models of devices

- Physical models of device degradation and performance variation caused by cosmic-ray environments
- Material and circuit models for space-compatible devices such as SiC, GaN, and organic semiconductors
- Thermal-transport simulations for space applications, handling integrated thermal management (solid, liquid, and radiation heat transfer)



Project's Objective：Hub Establishment Centered on a Sim. Platform

This project is a network-based initiative that, while centered in Kyoto as a core research hub, connects universities, research institutions, and companies across Japan, functioning as a hub for industry–academia–government collaboration beyond regional boundaries. Through this nationwide hub function based in Kyoto, the project brings together diverse stakeholders and continuously generates new businesses and communities originating from space experiments.

Space-Environment Simulation Platform

Material
(Raw materials･Production equipments)

Process
(Design･Process development)

Device
(Performance･Reliability)

"Semiconductor R&D"
Ind.–Acad.–Gov. Hub

- Large-scale comp.
- HRD･Exchange
- Funding･Circulation
- Space expt. support
- Regional Tech. Collab.
- Commercialization

Univ.･Res. Inst.	Corporations	JAXA	Local gov.	Banks･Investors
Sharing of research outcomes Community participation	Commercialization Community participation	Space environment utilization	Introd. of regional corps Community participation	Joint commercialization Funding support

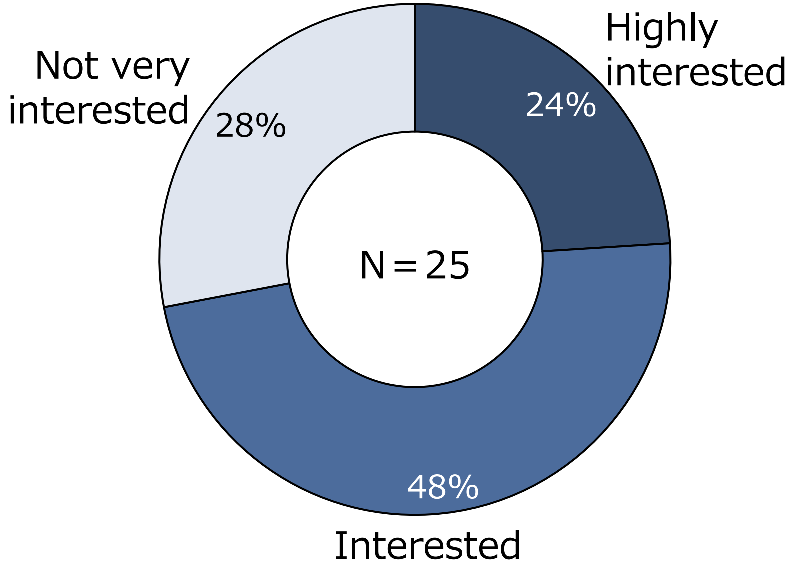
A network framework centered on Kyoto connecting univs & corps nationwide from tech. dev. stage.

This nationwide framework directly functions as a hub for industry–academia–government collaboration beyond regional boundaries.

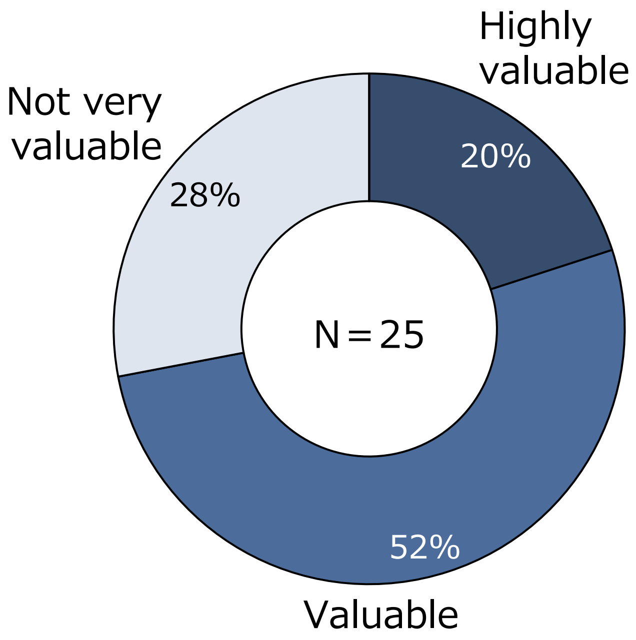
(Reference) Level of interest among potential user companies

A survey of 25 potential user companies showed that approximately 70% expressed strong interest in elucidating physicochemical phenomena under space environments, and similarly, more than 70% responded that simulations and databases would be “highly valuable.” In addition, about 70% indicated a willingness to consider paid use of the platform. These results confirm substantial latent demand in industry for such an infrastructure.

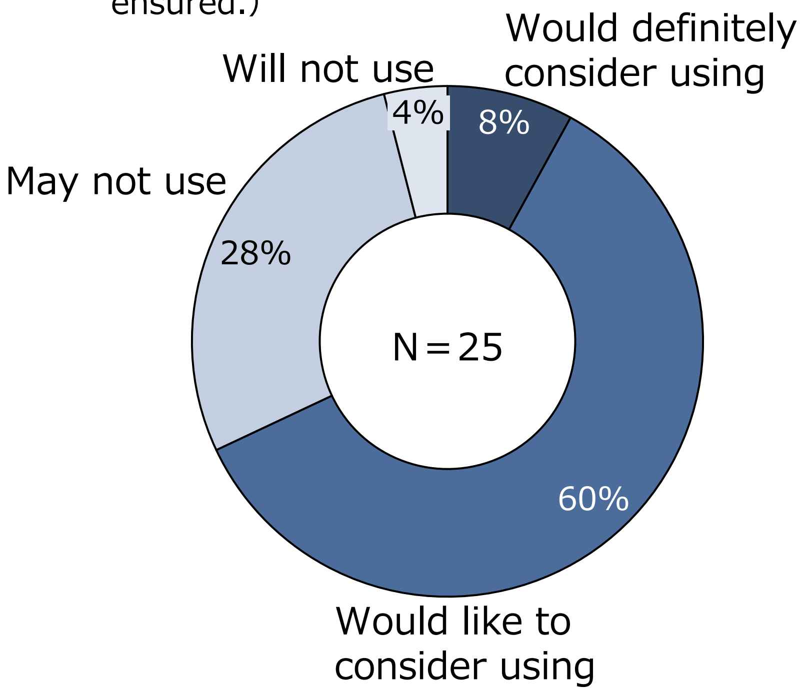
Q1 Please tell us the level of interest your company has in R&D aimed at elucidating physicochemical phenomena under space environments—such as microgravity—including the behavior of chemical solutions, dissolution/dispersion mechanisms, crystal growth, and related processes.



Q2 To what extent do you think the simulations/databases shown on the left would be useful or valuable for your company’s research and development?



Q3 Assuming that the simulations/databases shown on the left would contribute to solving your company’s challenges, to what extent would you consider using them on a paid basis?（With the premise that the confidentiality of your information is fully ensured.）

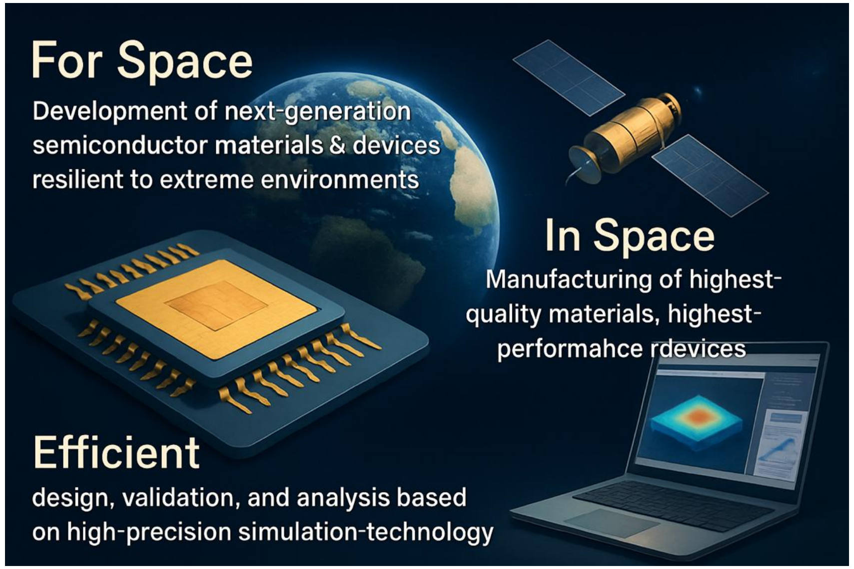


Project Targets

For Space: Development of next-generation semiconductor materials and devices resilient to extreme environments

In Space: Manufacturing of the highest-quality materials and highest-performance devices by utilizing the unique conditions of the space environment

Realization of highly efficient design, validation, and analysis grounded in high-precision simulation technologies applicable across all fields



"For-Space" Subjects

- Very high and low absolute temperature
- Large temperature gradient
- Severe thermal insulation by vacuum environment

→ **High temperature tolerance and heat release functionalities required in semiconductor materials and devices**

- High fluxes of high-energy protons, heavy ions, γ-rays, neutrons, electrons, and atomic oxygen

→ **High radiation tolerance and degradation modeling for proper maintenance required**

"In-Space" Subjects for Materials

In crystal growth, which is the most critical process in the synthesis of semiconductor materials, the utilization of the microgravity environment and highly clean conditions of outer space has been suggested to potentially improve material properties. For example, under microgravity, convection does not occur, enabling the production of more homogeneous materials, and contact with containers can be eliminated, thereby enhancing material purity.

- Because microgravity eliminates buoyancy and sedimentation forces, separation and distribution caused by differences in (mass) density can be suppressed, resulting in more homogeneous materials.
- Since convection does not occur, undesirable material transport can be reduced, contributing to enhanced material homogeneity.
- As thermal convection decreases, heat transfer is reduced, increasing the temperature gradient in the melt produced by heating, thereby facilitating unidirectional solidification.
- Because hydrostatic pressure is absent, lattice defects caused by hydrostatic stress can be reduced. This also contributes to precise spatial arrangement of materials.
- By minimizing contact between the material and its container, material purity can be improved.

From the fundamental research view aimed at acquiring knowledge useful for materials development:

- The reduction of thermal convection makes it easier to study solid–liquid interfaces.
- The reduction of gravity-induced hydrostatic pressure allows wetting and adsorption phenomena to be observed more prominently.

"In-Space" Subjects for Processes

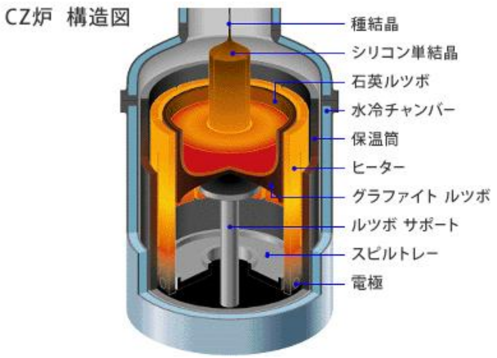
Environment	Total Pressure (Pa)	H_2O Concentration / Partial Pressure	O_2 Concentration / Partial Pressure	Atomic Oxygen Density	Particle (Dust) Density
Standard Atmosphere (Ground)	~1×10^5 Pa	1,000–3,000 Pa (RH50%)	~21,000 Pa	Negligible	~10^8–10^9 particles/m^3
Cleanroom (ISO 5–7)	~1×10^5 Pa	Several hundred to ~1,000 Pa	~21,000 Pa	Negligible	10^2–10^4 (ISO 5), 10^6–10^8 (ISO 7) particles/m^3
Ultra-High Vacuum (UHV) Chamber	10^{-6}–10^{-8} Pa	≤10^{-8} Pa	≤10^{-9} Pa	Negligible	Almost zero (desorbed molecules only)
Low Earth Orbit (LEO) 300–500 km	10^{-6}–10^{-4} Pa	~10^{-10} Pa	~10^{-8}–10^{-7} Pa	10^{10}–10^{12} atoms/m^3	~10^{-6}–10^{-4} particles/m^3
Geostationary Orbit (GEO)	10^{-9}–10^{-11} Pa	≪10^{-10} Pa	≪10^{-10} Pa	Almost zero	10^{-8}–10^{-6} particles/m^3

- Because gravity is extremely small, issues such as wafer or thin-film bending (which occur on the ground) can be eliminated, and it may become possible to process much thinner wafers.
- Unwanted contact with containers or other components inside processing equipment can be minimized.
- Aggregation and sedimentation of solutes in solution are significantly reduced, greatly improving the homogeneity and stability of the solution.

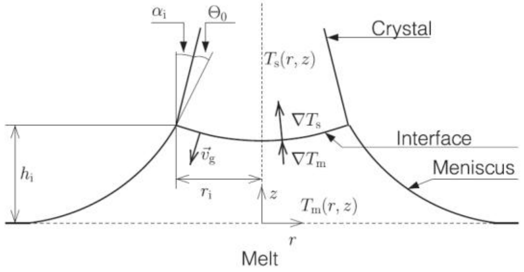
Example: Simulations for Semiconductor Crystal Growth Process

Calculated based on a mechanics- and heat-transport-based model of the single-crystal silicon (Si) ingot fabrication process.

The crystal growth rate under terrestrial conditions ($g = 9.8\ m/s^2$, $n = 1$) agrees with the typically reported value of 1 mm/min.
（demonstrating the validity of the model）



https://www.sumcosi.com/products/process/step_01.html



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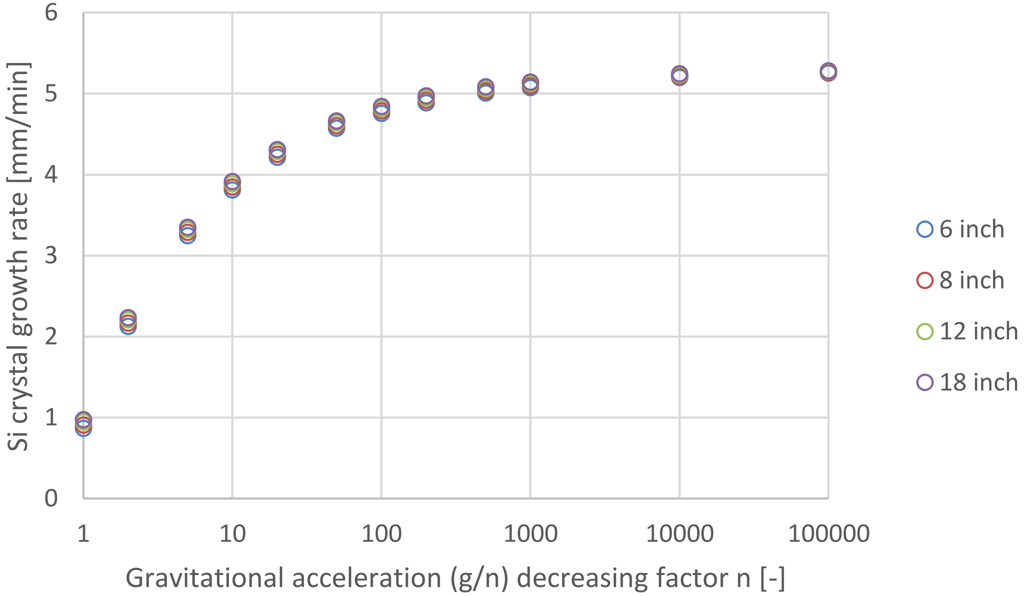
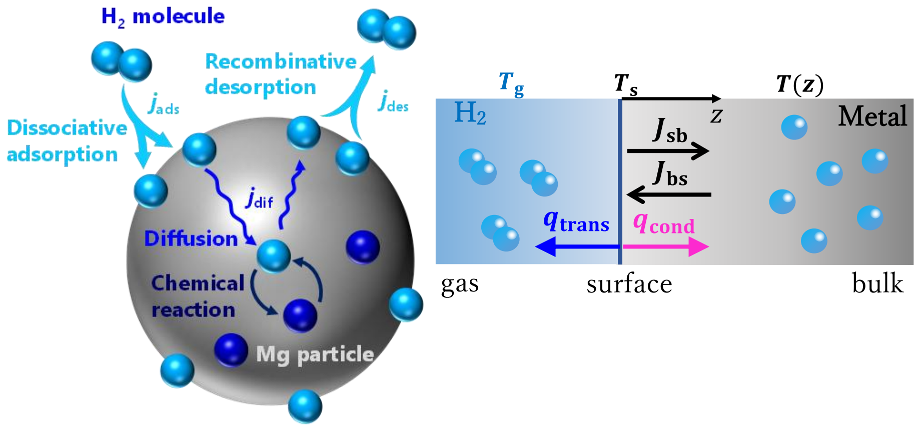


- In space environments, the crystal growth rate is expected to increase by several times.
- (Mechanism) Reduction of gravity → Elongation of the melt/solid interfacial meniscus
  → Decrease in the temperature gradient at the meniscus → Reduction of heat flux from the melt side
  → Enhancement of the crystallization rate, which is an exothermic process

Various Theoretical Simulation Schemes



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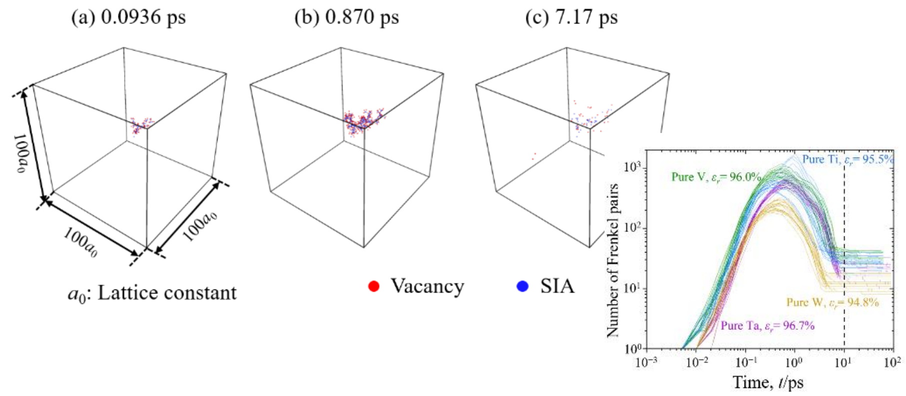
Macroscopic mass/heat transport・reaction models



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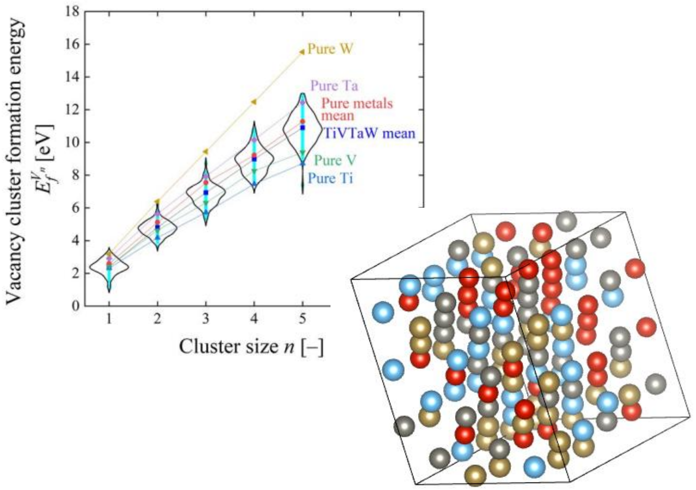
Molecular dynamics (MD) simulations



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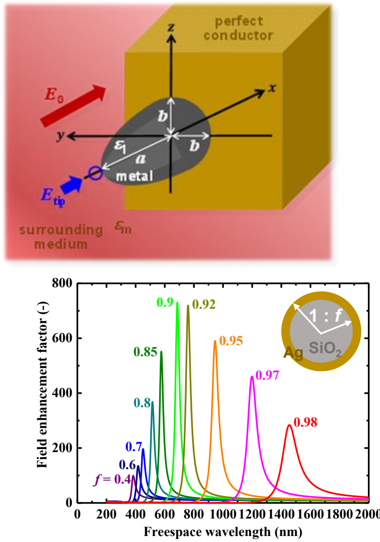
Density functional theory (DFT) calculations



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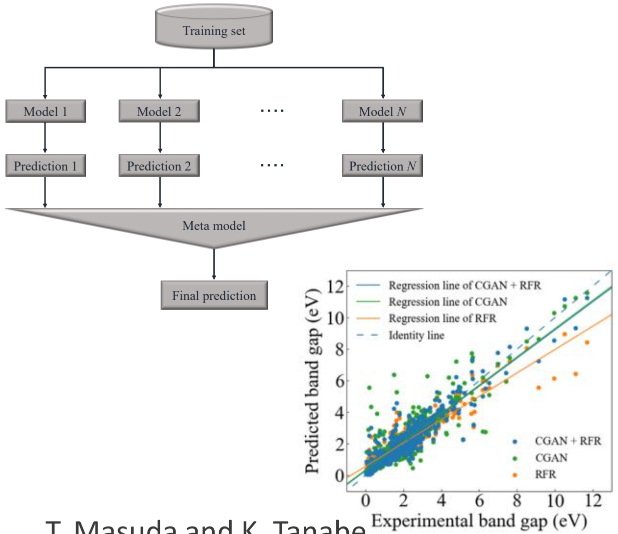
Electromagnetic field analysis



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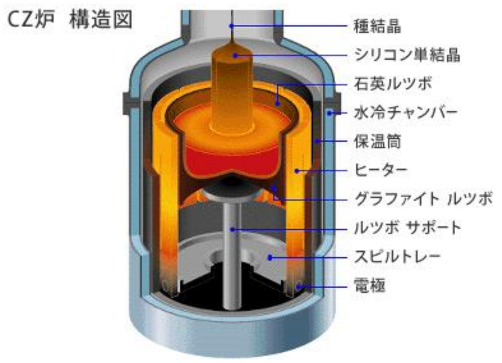
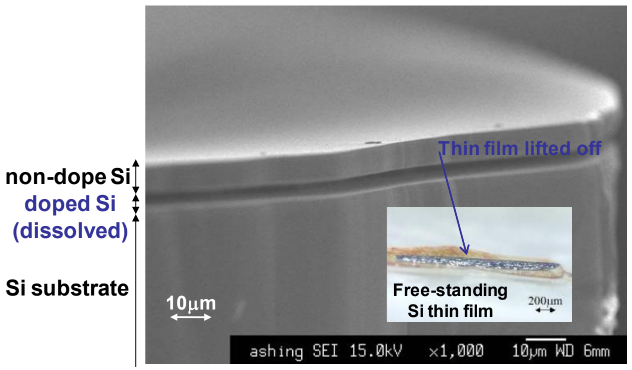
AI / machine learning

Potential Applications of Space Environment



https://www.sumcosi.com/products/process/step_01.html

Melt growth



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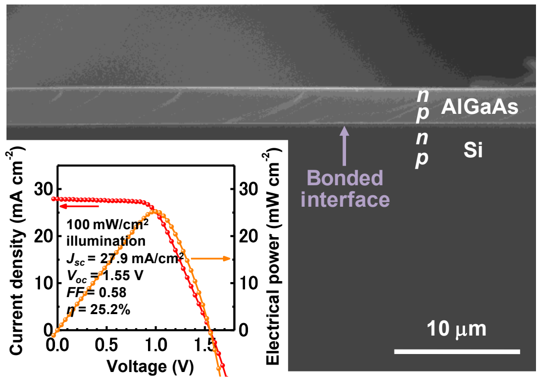
Gas-phase growth



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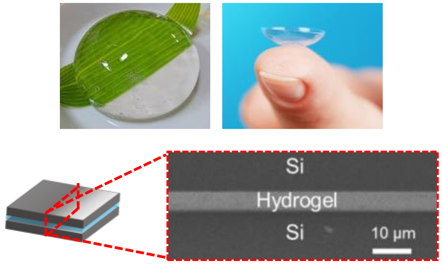
Wafer bonding



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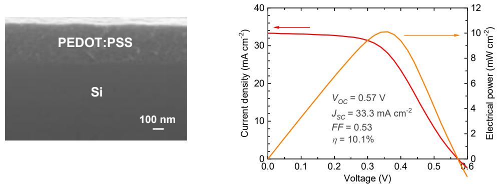
Wet processes



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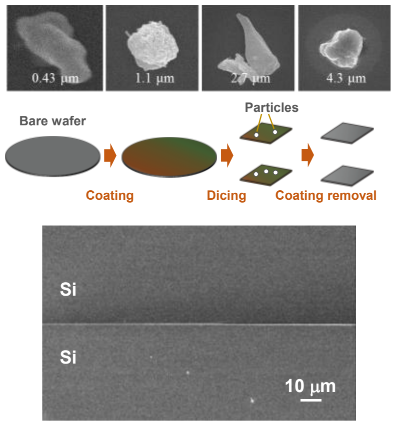
Anoxic environment use



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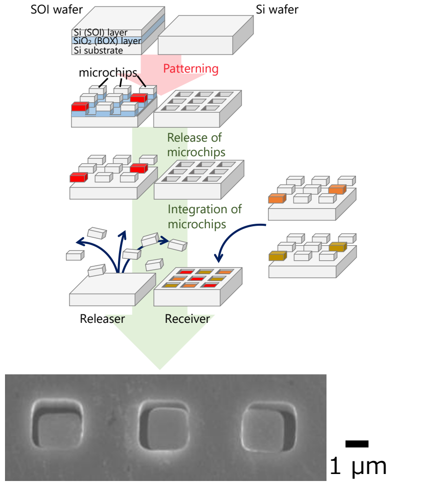
Particle control



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3-D self assembly

Issues & Targets: Irradiation Processes in Semiconductors

- To accurately simulate the effects of high-energy particles, it is necessary to take into account not only the energy distribution of the particles but also the fine structural details of the materials they traverse. Such modeling is highly complex and challenging.

- When cosmic rays collide with materials inside a device, secondary particles (such as electrons and positrons) are generated, which subsequently cause additional effects within the device. Numerical methods capable of tracking the behavior of these secondary particles and evaluating their impact are required. This significantly increases the computational load of simulations and necessitates high-performance computing resources to maintain accuracy.

- Because experimental data on the effects of cosmic radiation are limited, it can be difficult to compare simulation results with real-world data. In particular, data derived from device testing conducted in space are extremely scarce, making the acquisition of reference data for validating simulations a critical challenge.

Issues & Targets: Irradiation Processes in Semiconductors (Cont'd)

- There is a strong need to connect "materials simulations" of radiation damage with "device/circuit simulations" that predict practical performance changes and lifetime. This requires the integration of simulations across different scales, combining particle trajectory calculations and atomistic-level material simulations with high-dimensional simulations that reproduce the behavior of entire devices.

- As device miniaturization progresses and structural complexity increases, even the generation of a small number of charge carriers can lead to malfunction. Single-event effects in memories caused by neutrons, as well as single-event burnout (SEB)—short-circuit destruction of power devices induced by a single particle—have been extensively studied. Experimental observations of single-event effects in aircraft environments have also reported an increased occurrence of single-event upsets (SEUs), i.e., logic errors due to memory bit flips, at high altitudes.

- Although many devices based on novel principles, structures, and materials have been proposed, their irradiation effects remain largely unknown. Furthermore, phenomena such as ELDRS (Enhanced Low Dose Rate Sensitivity), in which total ionizing dose effects become more pronounced at lower dose rates even for the same absorbed dose, and irradiation-induced increases in leakage current in insulating films are well-documented fundamental effects. However, their physical mechanisms have not yet been fully elucidated, and further investigation is required to achieve high reliability in space-grade components.

Conclusions

- **Space environments provide an essential research platform for elucidating unresolved phenomena in semiconductor materials, processes, and devices**
  — Microgravity, radiation, and extreme thermal conditions enable insights that are difficult or impossible to obtain on the ground.

- **However, space experiments remain expensive and time-consuming, making continuous industrial utilization difficult**
  — This creates a structural gap where the need is high, but execution is challenging.

- **This project addresses the gap by developing an integrated simulation platform that scientifically reproduces space environments**
  — Multiscale modeling across materials, processes, and devices
  — Continuous accuracy improvement through linkage with space experiment data

- **A nationwide industry–academia–government hub centered in Kyoto will be established around this simulation platform**
  — Serving as a common infrastructure for R&D, commercialization, and human resource development

- **The platform will contribute not only to space R&D but also to advancing competitiveness and innovation in ground-based semiconductor industries**
  — Creating a new industrial ecosystem driven by the synergy of space and simulation technologies

Acknowledgement: Academic and industry members of the SX project, METI, Japan