



National Institute for Material Science



データ収集に関する研究者の取り組み、 データDOIへの期待

国立研究開発法人 物質・材料研究機構
情報統合型物質・材料研究拠点
国際ナノアーキテクトニクス研究拠点 (MANA)

知京豊裕

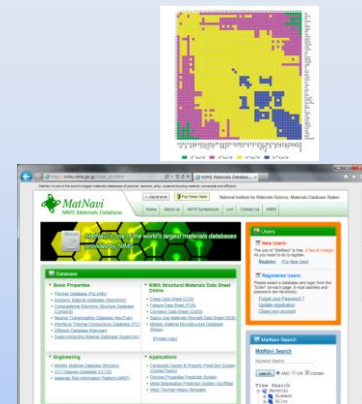
2017.3. 27 JaLC 「対話・共創の場」(第3回)



データ（選択）

演繹法

帰納法

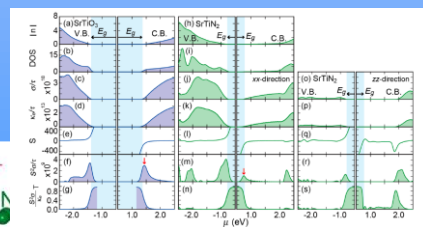


データベース

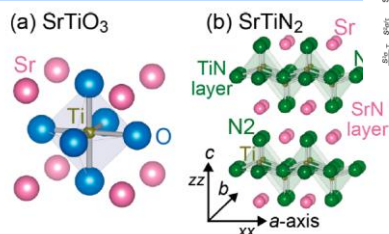


データ（蓄積）

材料合成



材料設計



材料合成

Materials database system : MatNavi

“MatNavi” is one of the world's largest materials databases provided by NIMS

See the web site,
http://mits.nims.go.jp/index_en.html

Database

Basic Properties

- ▶ [Polymer Database \(PoLyInfo\)](#)
- ▶ [Inorganic Material Database \(AtomWork\)](#)
- ▶ [Computational Phase Diagram Database \(CPDDb\) **NEW!**](#)
- ▶ [Computational Electronic Structure Database \(CompES\)](#)
- ▶ [Database of Promising Adsorbents for Decontamination of Radioactive Substances \(READS\)](#)
- ▶ [Neutron Transmutation Database \(NeuTran\)](#)
- ▶ [Interfacial Thermal Conductance Database \(ITC\)](#)
- ▶ [Diffusion Database \(Kakusan\)](#)
- ▶ [Superconducting Material Database \(SuperCon\)](#)

NIMS Structural Materials Data Sheet Online

- ▶ [Creep Data Sheet \(CDS\)](#)
- ▶ [Fatigue Data Sheet \(FDS\)](#)
- ▶ [Corrosion Data Sheet \(CoDS\)](#)
- ▶ [Space Use Materials Strength Data Sheet \(SDS\)](#)
- ▶ [Metallic Material Microstructure Database \(Kinso\)](#)

[\[Printed copy\]](#)

Engineering

- ▶ [Metallic Material Database \(Kinzoku\)](#)
- ▶ [CCT Diagram Database \(CCTD\)](#)
- ▶ [Materials Risk Information Platform \(MRiP\)](#)
- ▶ [FGMs Database](#)

Applications

- ▶ [Composite Design & Property Prediction System \(CompoTherm\)](#)
- ▶ [Polymer Properties Prediction System](#)
- ▶ [Metal Segregation Prediction System \(SurfSeg\)](#)
- ▶ [Interface Bonding Prediction System \(InerChemBond\) **updated**](#)
- ▶ [Weld Thermal History Simulator](#)

- ✓ “MatNavi” consists of about 20 database (polymer, inorganic materials, superconductivity, etc.) with high reliability.
- ✓ “MatNavi” provides data visualization tools and simple prediction simulator of material properties.

Materials Project (MIT)

Mission: Accelerating materials discovery through advanced scientific computing and innovative design tools.

Leader(s): Prof. G. Ceder

Budget: -

Collaborator(s): LBNL, Intermolecular, Inc.

MATERIALS PROJECT

A Materials Genome Approach

Accelerating materials discovery through advanced scientific computing and innovative design tools.

(2013年12月25日クリップ)

 e.g. explore Fe₂O₃ or Li-Fe-O pd

Search powered by **MOOGLE**

Database Statistics

35840 materials **17219** bandstructures

497 intercalation batteries **16135** conversion batteries

Database Statistics

54808

COMPOUNDS

25541

BANDSTRUCTURES

2091

LI INTERCALATION ELECTRODES

16128

LI CONVERSION ELECTRODES

論文のデータは
データ部のみ



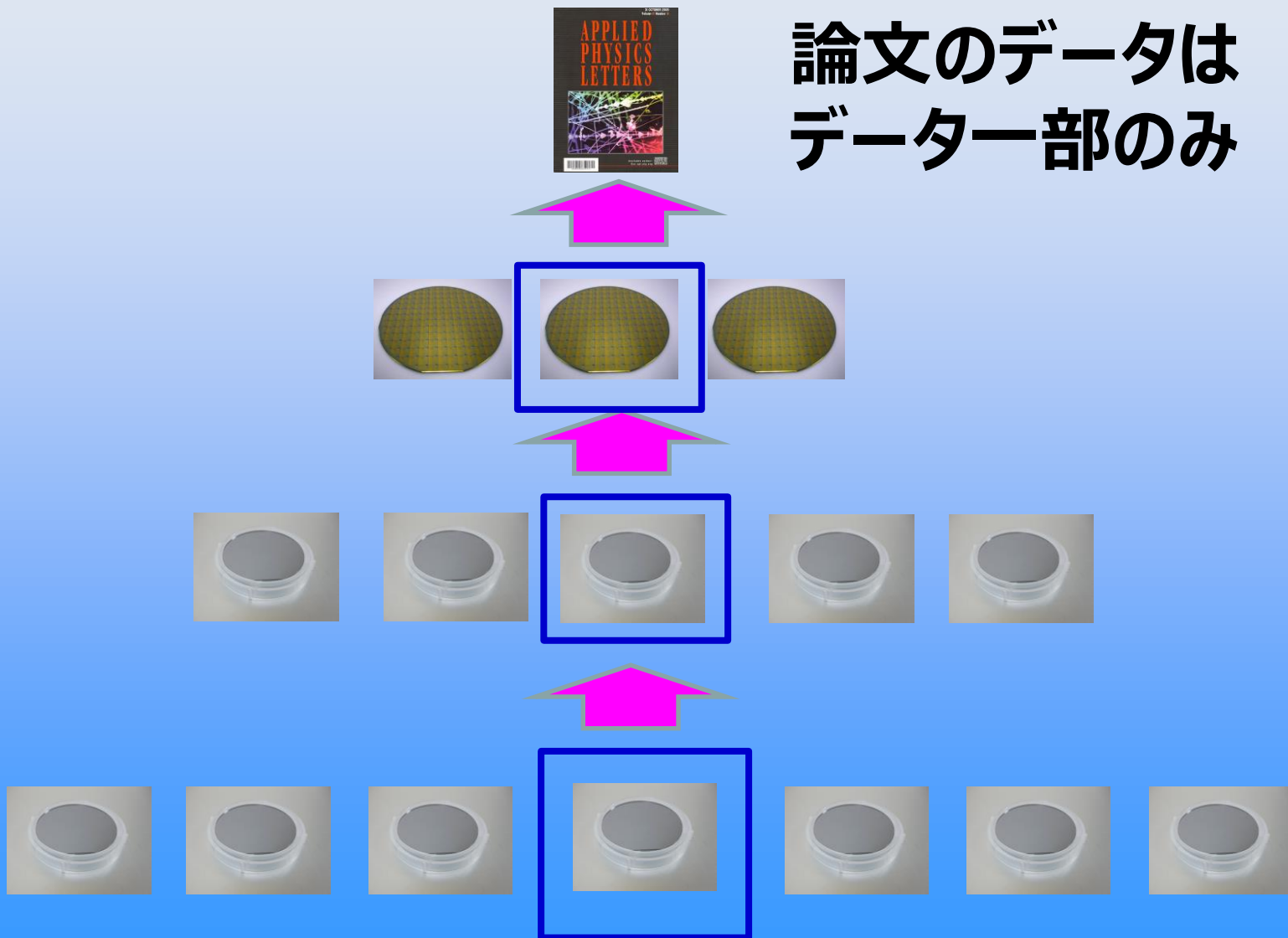
特性評価



材料評価

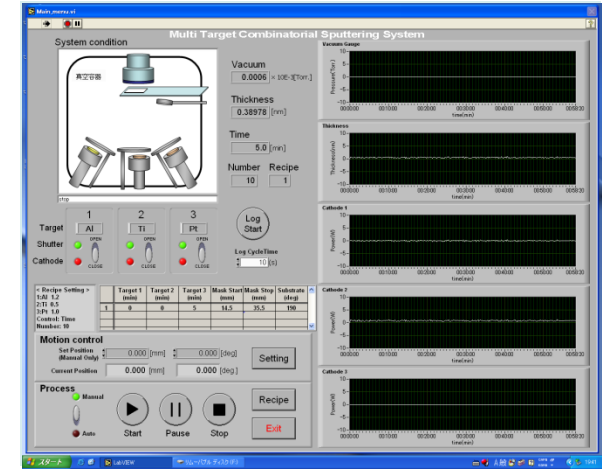
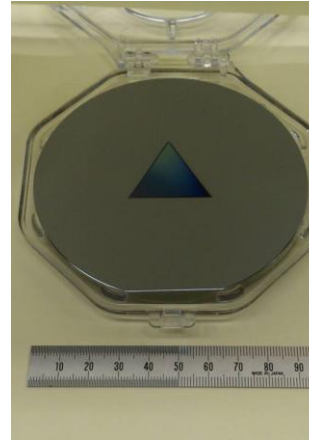


材料合成



High Throughput Experimentation for systematic data collection

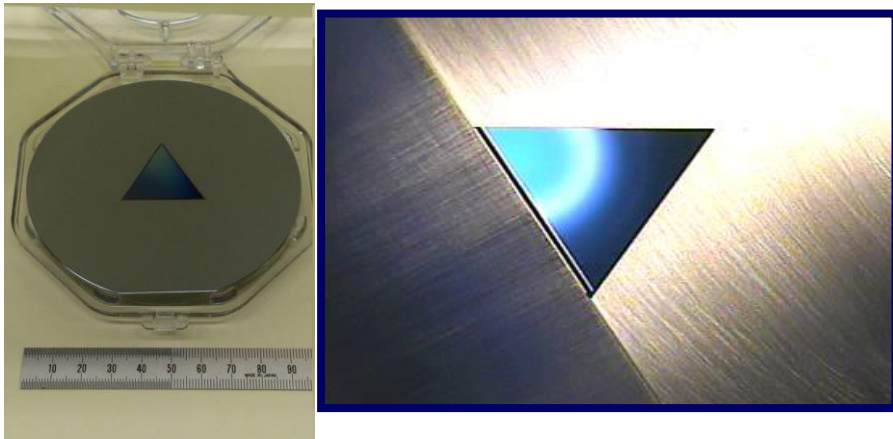
Multi-targets Combinatorial Sputtering system



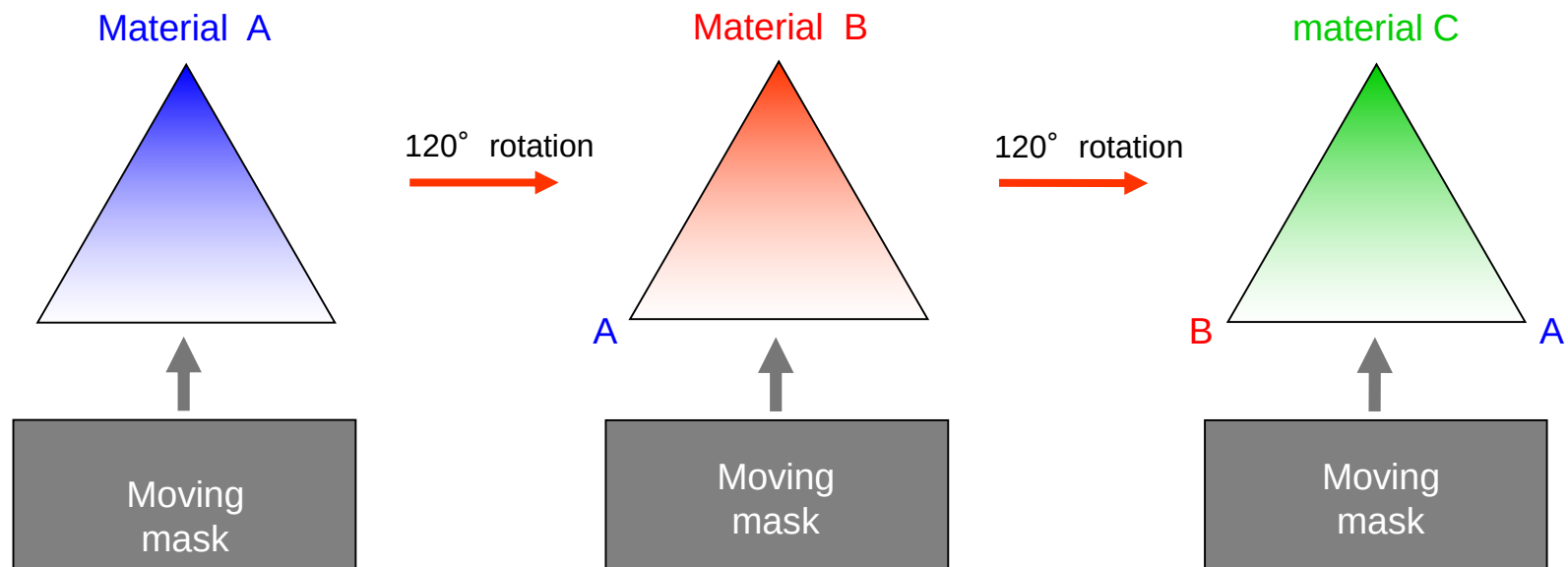
- ① GUI for every users
- ② automatic recording (date, condition, materials)
- ③ connection to Internet (Wireless LAN)

Automatic ternary alloying by combinatorial method

Composition spread

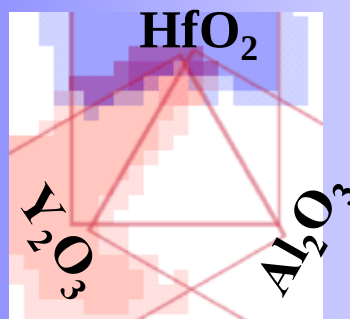
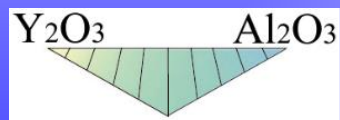
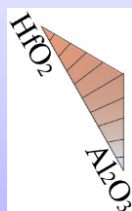
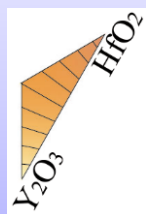
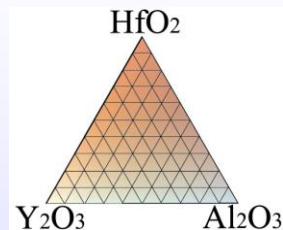


コンビスパッタ装置(コメット社製)



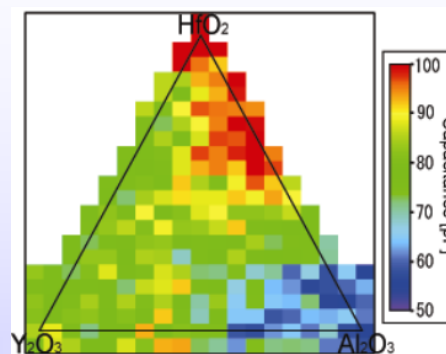
Repeat these synthesis process until getting the desired film thickness

Screening examples

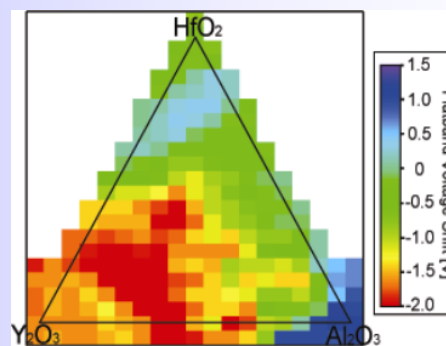


Structure mapping by XRD

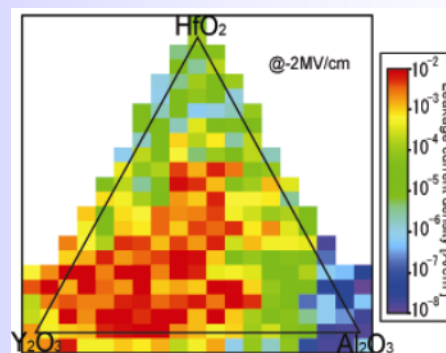
Dielectric property mapping



Flat band mapping



Leakage current mapping

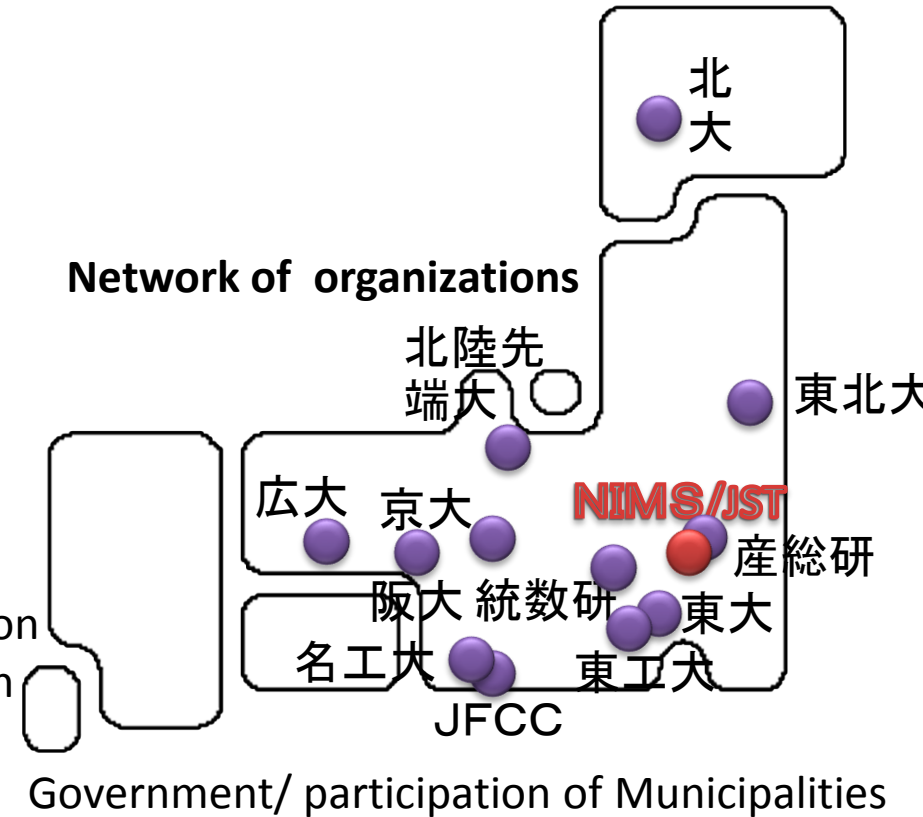


“all-Japan” by inter-regional cooperation

- NIMS/JST as hub organization
- Academia network
 - • • Hokkaido Univ., Tohoku Univ., Univ.Tokyo, TUT, JAIST, Nagoya Inst.Tech., Kyoto Univ., Osaka Univ., Hiroshima Univ., AIST, IMS, JFCC
- Translational research satellites

“all-Japan” by inter-sector cooperation

- Industry-government-academia cooperation
- A new scheme of multi-client collaboration

MI²I consortium (4/1/2016 ~)

- Collaboration in equal partnership of participants
- Sharing of information and achievements as possible

If you are interested → e-mail : mii-i@ml.nims.go.jp

Systematic data collection !

なぜDOIは必要か

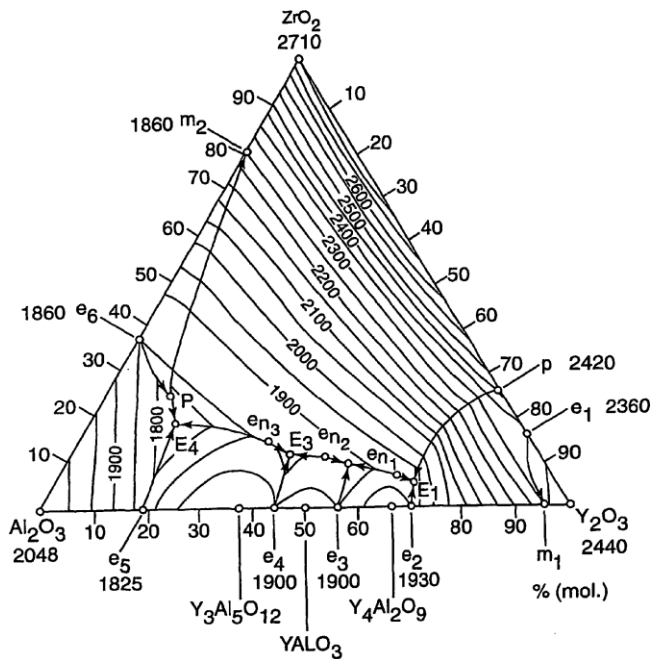
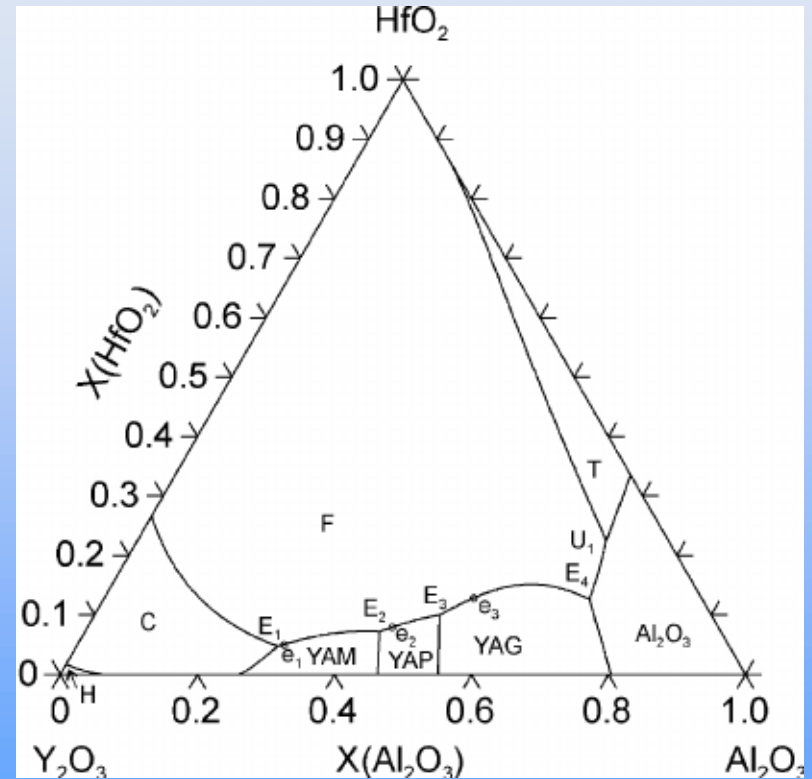


Fig. 4



特許から

学位論文から

現在：データのアドレスがない。

- 論文に載らないデータは捨てられる。
- どの装置で得たデータか不明のときがある。
- だれが作ったかも知りたい。（筆頭≠計測者）
- できれば、国際標準にしたい。



DOIに期待。

Digital platform for Materials Informatics



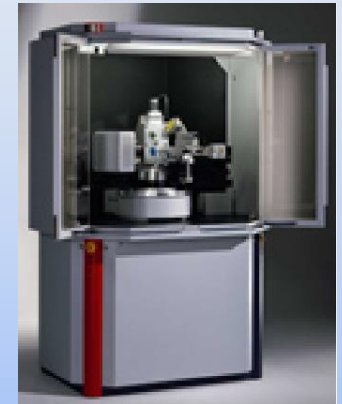
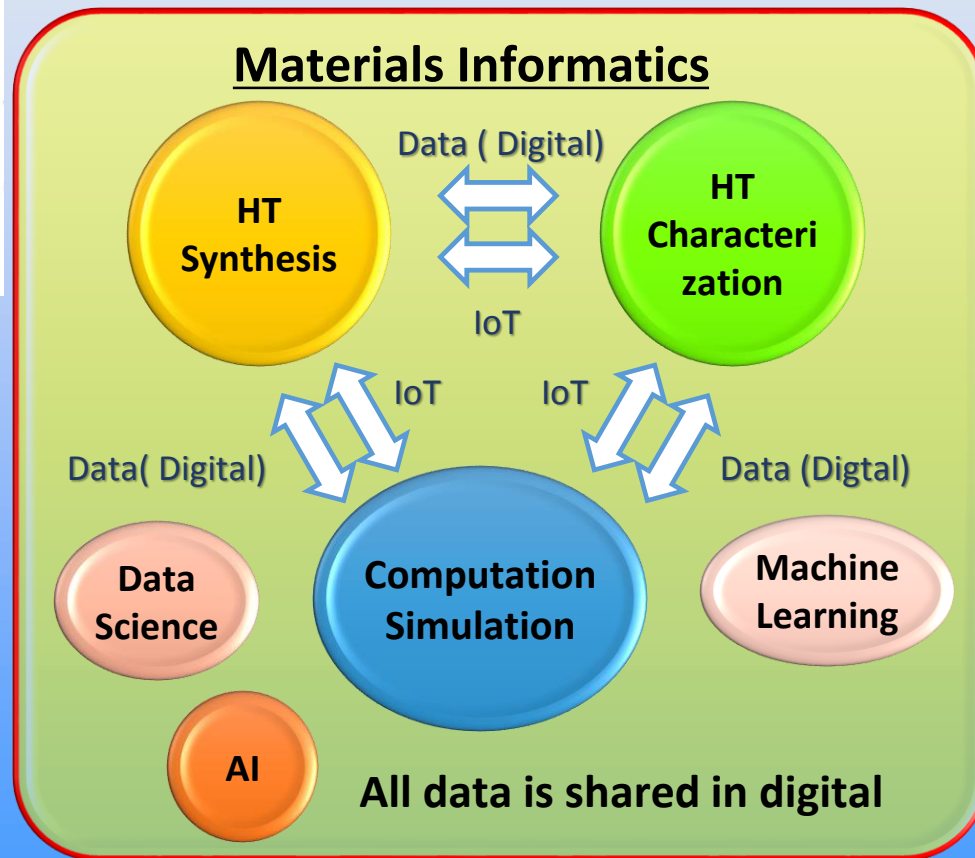
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実験装置



計算科学



評価装置
(構造)



評価装置
(特性)

How the future materials data base is ?

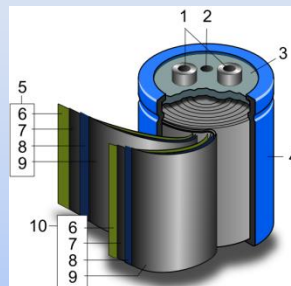
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Spicy type “visualization” in “Mat Cloud”



White paint



Capacitor



DSSC



UV
absorption

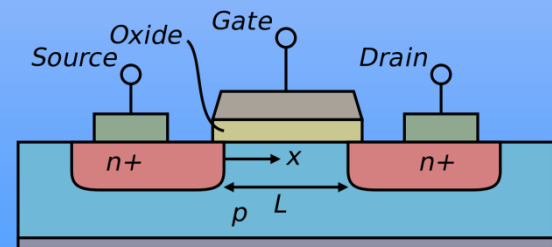
TiO_2

Al_2O_3

Nb_2O_5



Transparent conductive oxide



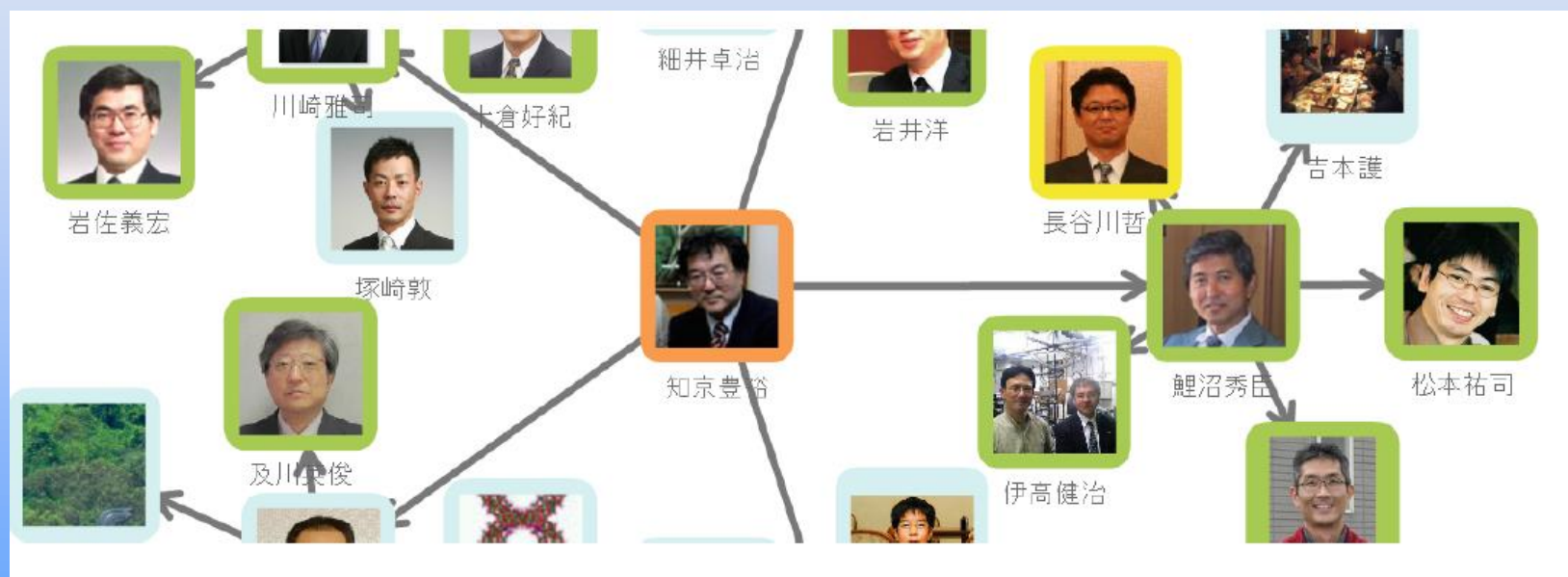
Gate insulator ($\epsilon=60$)

データの視覚化

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Spicy type “visualizing data”



結論

デジタル時代の材料科学のために、

- データを網羅的に集める体制
- データの関連付け
- データの視覚化

DOIはデジタル時代の材料科学に不可欠なツールとなる。

