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ナノ構造情報のフロンティア開拓 ―材料科学の新展開

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研究成果報告書

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領域代表者 田中 功  
京都大学・工学研究科・教授

## はしがき

材料の表面、界面、点欠陥等に局在した特徴的な原子配列や電子状態＝ナノ構造が材料特性に決定的な役割を担う例は数多くあります。

わが国は、ナノ構造における個々の原子を直接観察し、その定量的情報を直接的に得るための実験や理論計算、解析結果を具体的な材料設計・創出に活かす研究において、世界をリードする成果を上げてきました。

本領域研究は、このナノ材料科学を世界に先駆けてさらに開拓し、得られるナノ構造情報を合理的に活用するための方法論を確立させることを目的としました。

この研究目的を達成するためには、材料科学と他分野、とくに情報科学の密接な連携が不可欠でした。

一般に異分野の研究者どうしが意思疎通することは簡単ではありません。

本領域では、研究目標や専門用語を互いに共有することに意識して努めました。

その結果、当初の期待を超えるスピードで、質の高い融合研究の成果が上がりました。

また次世代を担う多くの若手研究者とそのネットワークが育成されました。

いま、まさに新しい材料科学の息吹を確実に感じることができます。

## 研究組織

### 計画研究

領域代表者 田中 功 (京都大学・工学研究科・教授)

(総括班)

研究代表者 田中 功 (京都大学・工学研究科・教授)

(国際活動支援班)

研究代表者 田中 功 (京都大学・工学研究科・教授)

研究分担者 柴田 直哉 (東京大学・工学系研究科・教授)

研究分担者 太田 裕道 (北海道大学・電子科学研究所・教授)

(計画研究 A01 ア班)

研究代表者 松永 克志 (名古屋大学・工学研究科・教授)

研究分担者 阿部 真之 (大阪大学・基礎工学研究科・教授)

研究分担者 中村 篤智 (名古屋大学・工学研究科・准教授)

研究分担者 豊浦 和明 (京都大学・工学研究科・准教授)

(計画研究 A01 イ班)

研究代表者 柴田 直哉 (東京大学・工学研究科・教授)  
研究分担者 藤平 哲也 (大阪大学・基礎工学研究科・准教授)  
研究分担者 石川 亮 (東京大学・工学系研究科・助教)  
研究分担者 栃木 栄太 (東京大学・工学系研究科・助教)  
研究分担者 溝口 照康 (東陽大学・生産技術研究所・准教授)

(計画班 A01 ウ班)

研究代表者 武藤 俊介 (名古屋大学・未来・システム研究所・教授)  
研究分担者 山本 剛久 (名古屋大学・工学研究科・教授)

(計画研究 A02 エ班)

研究代表者 田中 功 (京都大学・工学研究科・教授)  
研究分担者 吉矢 真人 (大阪大学・工学研究科・准教授)  
研究分担者 大場 史康 (東京工業大学・科学技術創成研究院・教授)

(計画研究 A02 オ班)

研究代表者 谷口 尚 (物質・材料研究機構・機能性材料研究拠点・グループリーダー)  
研究分担者 遊佐 斉 (物質・材料研究機構・機能材料研究拠点・主席研究員)  
研究分担者 村田 秀信 (横浜市立大学・国際総合科学部・助教)  
研究分担者 宮川 仁 (物質・材料研究機構・機能材料研究拠点・主任研究員)  
研究分担者 吉田 英弘 (物質・材料研究機構・機能材料研究拠点・主幹研究員)

(計画研究 A02 カ班)

研究代表者 太田 裕道 (北海道大学・電子科学研究所・教授)  
研究分担者 平松 秀典 (東京工業大学・科学技術創成研究院・准教授)

(計画研究 A02 コ班)

研究代表者 津田 宏治 (東京大学・新領域創成科学研究科・教授)  
研究分担者 志賀 元紀 (岐阜大学・工学部・准教授)  
研究分担者 鹿島 久嗣 (京都大学・情報学研究科・教授)

(計画研究 A03 キ班)

研究代表者 北岡 諭 (ファインセラミックスセンター・材料技術研究所・主席  
研究員)

研究分担者 森分 博紀 (ファインセラミックスセンター・ナノ構造研究所・主席  
研究員)

(計画研究 A03 ク班)

研究代表者 菅野 了次 (東京工業大学・科学技術創成研究院・教授)

研究分担者 田村 和久 (日本原子力研究開発機構・原子力科学研究部門・研究副  
主幹)

研究分担者 平山 雅章 (東京工業大学・物質理工学院・准教授)

研究分担者 鈴木 耕太 (東京工業大学・物質理工学院・助教)

(計画研究 A03 ケ班)

研究代表者 高草木 達 (北海道大学・触媒科学研究所・准教授)

研究分担者 原 賢二 (東京工科大学・工学部・教授)

研究分担者 清水 研一 (北海道大学・触媒科学研究所・教授)

(公募研究 第一期)

研究代表者 一杉 太郎 (東北大学・原子分子材料科学高等研究機構・准教授)

研究代表者 王 中長 (東北大学・原子分子材料科学高等研究機構・准教授)

研究代表者 高橋 幸生 (大阪大学・工学研究科・准教授)

研究代表者 永田 賢二 (東京大学・新領域創成科学研究科・助教)

研究代表者 鹿島 久嗣 (京都大学・情報学研究科・教授)

研究代表者 本多 淳也 (東京大学・新領域創成科学研究科・助教)

研究代表者 志賀 元紀 (岐阜大学・工学部・助教)

研究代表者 竹内 一郎 (名古屋工業大学・工学研究科・教授)

研究代表者 池野 豪一 (大阪府立大学・21世紀科学研究機構・講師)

研究代表者 東 正樹 (東京工業大学・応用セラミックス研究所・教授)

研究代表者 藤田 晃司 (京都大学・工学研究科・准教授)

研究代表者 横井 俊之 (東京工業大学・資源化学研究所・助教)

研究代表者 舟窪 浩 (東京工業大学・総合理工学研究科・教授)

研究代表者 柳田 剛 (九州大学・先導物質化学研究所・教授)

(公募研究 第二期)

研究代表者 高橋 康史 (金沢大学・電子情報学系・准教授)

研究代表者 高橋 幸生 (大阪大学・工学系研究科・准教授)

研究代表者 水野 正隆 (大阪大学・工学系研究科・准教授)  
 研究代表者 Packwood, Daniel (京都大学・iCeMS・講師)  
 研究代表者 本多 淳也 (東京大学・新領域創成科学研究科・講師)  
 研究代表者 竹内 一郎 (名古屋工業大学・工学系研究科・教授)  
 研究代表者 島川 祐一 (京都大学・化学研究所・教授)  
 研究代表者 中平 敦 (大阪府立大学・工学系研究科・教授)  
 研究代表者 池野 豪一 (大阪府立大学・工学研究科・准教授)  
 研究代表者 舟窪 浩 (東京工業大学・総合理工学研究科・准教授)  
 研究代表者 北條 元 (九州大学・装具李王学研究院・准教授)  
 研究代表者 藤井 孝太郎 (東京工業大学・理工学研究科・助教)  
 研究代表者 山崎 仁丈 (九州大学・稲盛フロンティア研究センター・教授)  
 研究代表者 黒川 修 (京都大学・工学研究科・准教授)

交付決定額 (配分額)

	合計	直接経費	間接経費
平成 25 年度	324,610,000 円	249,700,000 円	74,910,000 円
平成 26 年度	275,990,000 円	212,300,000 円	63,690,000 円
平成 27 年度	292,370,000 円	224,900,000 円	67,470,000 円
平成 28 年度	295,750,000 円	227,500,000 円	68,250,000 円
平成 29 年度	200,720,000 円	1,54,400,000 円	46,320,000 円
総計	1,389,440,000 円	1,068,800,000 円	320,640,000 円

## 1. 研究領域の目的及び概要

### 【我が国の学術水準の向上・強化】

本領域研究は、我が国が世界の優位にある材料科学分野をさらに強化するために立案された。

材料特性において、結晶の表面、界面、点欠陥等に局在した特徴的な原子配列や電子状態＝ナノ構造が決定的な役割を担う例は極めて多い。近年になりナノ構造における個々の原子を直接観察し、その定量的情報を直接的に得るための実験および理論計算に格段の進歩があり、我が国において世界を先導する成果が数多く上げられた。本領域研究は、このナノ材料科学分野の最先端の開拓にさらなる弾みを付けるとともに、獲得されるナノ構造情報を具体的な材料設計・創出に活かすべく情報の統合化を強力に進めること、すなわちナノ構造情報を活用した普遍的な材料開発原理の構築を目的とする。そのために、材料科学、情報学、応用物理、固体化学、触媒化学など様々な分野で世界に誇る成果をあげている若手・中堅研究者を中心としたメンバーが結集し、一体となって研究が進め、新しい材料科学の奔流を創り出す。

本領域研究には、ナノ材料科学のフロンティア開拓とナノ構造情報の活用という2つの明確なアプローチがある。これらを密接連携させ、領域の目的を達成するために、図1に示す3つの研究項目を設けた。**研究項目 A01：ナノ材料科学のフロンティア開拓**においては、高品質かつ多様なナノ構造情報を獲得し、領域内での融合・共同研究に供するために実験および理論計算の最先端技術の開拓を進める。具体的には最先端の透過型電子顕微鏡や原子間力顕微鏡により、ナノ構造における原子配列や元素分布、状態解析を定量的に行うとともに、高精度第一原理計算を実施する。**研究項目 A02：ナノ構造情報シンセシスによる機能設計・探索**では、研究項目 A01 において獲得されたナノ構造情報を具体的な材料創製に活かすべく、情報の統合化を、統計熱力学および情報学の学問体系に立脚して強力に進める。そして、高温・高温プロセスおよび原子層制御によってナノ構造をビルトインしたモデル材料を創製する。**研究項目 A03：ナノ構造デザインに基づく新しい材料創製**では、研究項目 A01 と A02 の成果をもとに獲得されたナノ構造デザインの結果を、新しい材料創製を合理的・効率的に行うことを通じて実証する。具体的には、領域内で3つの材料課題、すなわち機能性セラミックス材料、固体イオニクス材料、触媒材料を設定し、それぞれについて、領域全体で一丸となって研究を進める。具体的に重要な材料創製に結実させるために、3つの課題それぞれについて材料創製のエキスパートを、研究項目 A03 における計画研究代表者として配置する。このようにナノ構造情報を積極的に活用した材料開発の流れを3つの異なる材料分野において構築することにより、普遍的な材料開発原理が導かれ、材料科学への新展開が産まれると期待される。

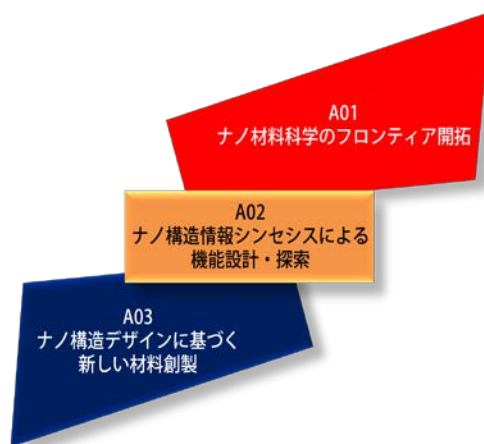


図1 ナノ構造情報を活用した普遍的な材料開発原理の構築のための領域の構成

### 【研究の学術的背景：応募領域の着想に至った経緯】

伝統的な材料技術に近代科学が適用されたのは20世紀半ばである。化学熱力学や固体物理学の材料分野への適用が進み、学問体系に基づいて実験結果を統合・整理することで、

自由エネルギーや物性値の化学組成や構造への依存性といった多様な**材料情報**が蓄積された。これらの情報を活用することで、材料技術が大きく進展し、技術革新が科学の一層の発展を促した。

この歴史の中で、結晶の表面、界面、点欠陥等に局在した特異なナノ構造が、材料特性に決定的な役割を担う例が数多く見出された。21世紀になり、このようなナノ構造についての情報を直接的に得るための実験・理論計算手法が格段に進歩しつつある。これらの研究進展により、これまで未知であった**ナノ構造と機能の関係=ナノ構造情報**を直接かつ定量的に獲得する方が拓かれた。その結果として構築されつつあるのが**ナノ材料科学**と呼ばれる分野であり、今後のさらなる発展が期待されている。材料設計・創出という観点に立つと、ナノ材料科学の応用分野の重要性は明確である。すなわちナノ構造情報についての普遍的な原理をもとに、デザインされた材料創出を合理的・効率的に行うことである。これは、従来の「勘と経験」に基づいて行われてきた材料研究に革新的な進歩をもたらすものと期待される。

一方で、実験や理論計算で得たナノ構造情報そのままでは、材料創出への応用範囲は極めて限定的である。個別の材料についての、いわゆるアナリシス型研究開発である。これに対し、普遍的な材料開発原理を導き出すためには、情報の統合化=シンセシスを、統計熱力学および情報学という学問体系に立脚して強力に進めるという研究が不可欠である。本領域研究の目標はまさにその点にあり、それは諸外国にも例を見ない独創的なものである。

最近、米国を中心に大容量計算機を利用して膨大な材料情報を整理し、材料開発に役立てようという大型プロジェクトが開始している。たとえば米国の *Materials Genome* と呼ぶ研究展開である。このような米国での研究展開と本領域研究とは、以下の2点において決定的に異なる。第一は、本領域研究がナノ構造情報に焦点を合わせている点である。本領域代表者らは、新材料設計・創出に情報学手法を適用することによって生じるパラダイムシフトは、精確なナノ構造情報抜きには達成できないと考えている。第二は、本提案が実績あるナノ材料科学のフロンティア開拓研究を中核に置いている点である。これにより最新の成果を直ちに機能設計・探索に応用することが可能となっている。

**【研究の学術的背景：応募時までの研究成果を発展させる場合にはその内容等】**

多様な材料系において、その特徴的な機能は、純物質単結晶の性質ではなく、結晶内部あるいは、表面、粒界、格子欠陥などに局在する特定元素=**ナノ機能元素**によって発現したものである。このナノ機能元素を対象にナノ計測実験、ナノプロセス実験、そして第一



図2 本領域における新学術創出のアプローチ

原理計算の3つのグループが、2007～2011年度に実施された特定領域研究「機能元素のナノ材料科学」において密接な共同研究を行った。その結果、この3分野連携の重要性が強く認識され、材料のナノ構造と機能の関連性についての定量的知見＝**ナノ構造情報**を獲得するための確固たる礎が築かれた。この特定領域研究は、事後評価として、**A+**（研究領域の設定目的に照らして、期待以上の研究の成果があった）という極めて高い評価を得た。今回の新学術領域研究は、この特定領域研究の成功体験と大きな研究成果に立脚し、その中で育成された若手・中堅研究者が中心メンバーとなり、材料創製や情報学などの分野から新しい研究者を招き入れて計画立案された。すでに高い実績を持つナノ材料科学のフロンティア開拓を、さらに弾みを付けて強化するとともに、獲得されるナノ構造情報を材料設計に活用するという材料科学の新展開を目指すものである。特定領域研究と本領域研究との発展的な関係については、図2に模式的に示したとおりである。また本領域研究における**ナノ材料科学のフロンティア開拓とナノ構造情報の活用**という2つのアプローチが、新しく参加した材料創製や情報学の研究者によって1つに束ねられ、それが新学術の展開を構成するという本研究の狙いも、図2に表現されている。

## 2. 研究領域の設定目的の達成度

### 研究領域全体としての達成度

#### 1. 設定目的の達成度

本領域は**ナノ材料科学のフロンティア開拓とナノ構造情報の活用**という2つのアプローチを密接連携させて**ナノ構造情報を活用した普遍的な材料開発原理の構築**という材料科学の新展開を導くことを目的として実施された。領域内に設定した3つの材料課題、すなわち機能性セラミックス材料、固体イオニクス材料、触媒材料を**コモンサブジェクト（CS課題）**と名付け、多様な材料に関わる様々な材料科学の課題に対し、領域メンバーがナノ構造情報を活用して材料開発原理を構築するという**共通の志**を持って融合・共同研究を行なうように工夫した。また各班の役割を後述の①から⑤の研究目的に具体化し、それに沿って重点的に研究を進めた。その結果、高品質かつ多様なナノ構造情報の獲得から材料開発に繋がる一貫した流れを、個別材料に留まらず多様な材料に対する普遍的な材料開発原理として構築できただけでなく、それを新材料創製として実証することができた。これを可能にするために、本領域では**材料科学分野と情報学分野の強固な連携**に特段の措置を講じた。具体的には期間前半に**6名**の情報分野の研究者を公募研究として採用し、領域代表者を中心として若手研究者によるタスクフォースを形成して活発な活動を行った。その結果、研究目標や専門用語が共有され、融合研究が活性化された。期間後半では、タスクフォースによる材料科学と情報学との融合研究をさらに強化・加速するために、研究項目**A02**に計画研究を1つ追加し、既設の計画研究と密接に協力してナノ構造情報に基づいた機能探索への適用的を絞った新しい機械学習法の開発や応用研究を実施した。これによりナノ材料科学における研究課題の情報学的な問題設定と普遍的特徴量の導出として成果を上げることができ、分野融合の進んだ「**新学術領域**」の構築に貢献できた。**材料科学と情報学の融合論文**は、期間前半には**8報**であったが、領域内研究者の相互理解が深まるにつれて、加速度的に領域内融合研究が進展し、最終的に本領域研究期間内に**33報**出版するに至った。この**A02**の強化により、**A01**で開拓された最先端技術によるナノ構造情報を**A03**における新しい材料創製につなげるという普遍的な材料開発原理としての一貫した流れが、期間後半において大きく加速された。具体的な成果としては、粒界制御した多結晶アルミナ耐環境セラミックスの創製、世界初のヒドリド（水素化物）イオン伝導酸水素化物と電気化学デバイスの創製、新しい金属担持触媒材料の創製などを上げることができる。このように、



ナノ構造情報を活用した普遍的な材料開発原理の構築という領域研究の目的は、実証の段階まで到達でき、当初計画が100%以上に達成できただけでなく、様々な新材料創製に成功という期待以上の成果があったと自己評価している。

## 2. 領域運営の達成度

### 2-1 融合領域の将来を担う若手人材の育成

計画研究班と公募研究班が融合・共同研究を実施するだけでなく、協力して将来を担う若手人材の育成に力を注いだ。毎年、合宿形式で『若手の会』を開催したほか、領域内他班への若手人材の相互訪問を奨励し、その延長線として、1年程度の大学院生・若手研究者の領域内他班への長期滞在プログラムを4件実施した。この活動を通して、個々の専門性が深まるだけでなく、異分野の理解や交流が進み、若手の人的ネットワークが創出できた。また情報学の専門家の補助なしに材料科学と情報学を融合した研究を推進できる人材が輩出できた。本領域研究は平成25年に開始し、平成27年と29年に開始した材料インフォマティクス関連のJST事業においては、本領域の若手メンバーが研究代表者としてCRESTが2名、さががけが8名採択され活躍している。当初計画は100%以上に達成できただけでなく、融合領域研究を次世代に確実に継承できたと自己評価している。

### 2-2 国際活動

総括班を司令塔として国際活動を積極的に進めた。平成27年度から3年間は国際活動支援経費を受け、総括班の国際活動推進委員会において選抜した研究者の長期海外派遣と領域内への受入を実施した。国際的な情報発信として、世界各国において領域メンバーによるレクチャーを実施したが、その成果を領域代表者が編集者となってまとめ、平成30年2月にSpringer社よりNanoinformaticsという表題で印刷版と電子版を同時にオープンアクセス出版した。同社では、出版後20か月で2万ダウンロードが企画成功の判断基準となっているが、同書は出版後3か月で目標を達成した。さらに領域内の多数の材料科学研究者が情報学の国際会議で、また情報学の研究者が材料科学の国際会議で招待講演を行っている。これらは、本領域での材料科学と情報学の融合研究成果への世界中からの注目度の高さを客観的に示すものである。これらの事実に基づき、国際活動についても当初計画は100%以上に達成できたと自己評価している。

### 2-3 国内活動・アウトリーチ活動

専門分野の研究者に向けて毎年1回公開シンポジウムを開催し、最新の研究内容をNews Letterとして配布した。そのほか、国内の学協会でのシンポジウムや講演会、基礎講座、特集雑誌の刊行を積極的に行った。アウトリーチ活動としては、一般市民や中高生を対象とした領域研究内容の紹介を「京都大学アカデミックデイ」において毎年実施した。当日の説明やポスター作成は、本領域参加機関の大学院生が担当した。これは説明する側にとっても、研究の社会的意義を再確認する良い機会となった。これら国内活動・アウトリーチ活動についても、当初計画は100%以上に達成できたと自己評価している。

## 研究項目ごとの達成度

### 研究項目 A01 ナノ材料科学のフロンティア開拓（計画3班、公募1期3班、2期3班）

目標：最先端の電子顕微鏡、回折・分光並びに第一原理計算を駆使した原子・電子スケールでのナノ構造評価・解析手法のフロンティアを世界に先駆けて深く広く開拓し、獲得した多様な高品質ナノ構造情報データを融合・共同研究に供する。

#### ①高品質なナノ構造情報の取得技術の開拓

表面、界面、添加元素などのナノ構造の解析手法やナノ電子分光における情報処理技法の開発と応用などの多くの革新的成果が得られた。具体的には、1 Å以下の空間分解能を有する走査型透過電子顕微鏡（STEM）を用いて粒界の原子構造やそこに濃化する不純物・溶質原子の存在を実空間で直接観察する手法を確立し、これと第一原理計算を併用することにより、セラミックス粒界における溶質偏析挙動を原子レベルで解明することに成功し

た。そして獲得したナノ構造情報データに基づき、CS 課題である粒界制御した耐環境セラミックスの創製に成功した。また酸化チタン表面に担持した金および白金の単原子吸着構造を直接観察し、その構造の起源を第一原理計算により解析する手法を確立した。このナノ構造情報データを情報学の観点から解析した結果、CS 課題である新しい金属担持触媒材料の創製が導かれた。

### ②情報学・統計学を活用したハイパー電子顕微鏡分光法の開発

ナノ構造に対し、サブナノメートルサイズの電子プローブを用いた走査イメージ (STEM 像) と電子エネルギー損失分光 (EELS) などの分光分析データを同時測定し、情報学との融合研究を行って非負値テンソル分解 (NTF) 分解法を開発した。これは得られた三次元以上の数値列 (テンソル) としてのビッグデータから先験的情報なしに構成する少数の特徴量を見出すことを目的としたものである。本研究の結果、異相界面で化学状態を示すスペクトルが重なっているものを分離表示したり、信号/ノイズ比の小さいデータから重要な情報を抽出することが可能となった。この手法を CS 課題である生体親和性の高いセラミックス材料の表面解析や磁性材料における格子欠陥の磁性解析に適用し、獲得したナノ構造情報をもとに、新材料創製の設計指針が導かれた。

### 研究項目 A02 ナノ構造情報シンセシスによる機能設計・探索 (計画 4 班, 公募 1 期 6 班, 2 期 4 班)

目標: 研究項目 A01 において獲得された高品質なナノ構造情報を具体的な材料創製に活かすために、情報の統合化を、統計熱力学および情報学の学問体系に立脚して強力に進める。そして、高圧・高温プロセスおよび原子層制御によってナノ構造をビルトインしたモデル材料を創製する。

### ③ナノ材料科学における研究課題の情報学的問題設定と普遍的特徴量の導出

ナノ構造情報を具体的な材料創製に活かすためには、ナノ材料科学における研究課題を情報学の言葉で表現して問題設定すること、そしてナノ構造を表現する普遍的特徴量を導出することが最重要であるという認識を得た。これらの認識のもと、総括班主導により形成したタスクフォースにおいて、材料科学と情報学の研究者が高い頻度で議論を重ねることで、種々の材料科学の現象を情報学の問題として設定することに成功した。またナノ構造情報を記述する特徴量の導出にも取り組み、ナノ構造の特徴量として、粒界構造、点欠陥・伝導イオンや表面構造を記述する幾つかの普遍的な特徴量を提案した。さらに構造のみならず、ナノ構造に含まれる元素の記述方法、元素および構造を同時に記述する特徴量を提案するに至った。これらの成果は世界的にも類のない、いわば本領域メンバーの独創的な融合研究成果である。具体的には、セラミックス粒界構造の高効率探索、第一原理計算とベイズ最適化による複雑なイオン伝導経路の高効率探索、仮想スクリーニング法・推薦システムによる高効率な新物質・新機能の発見、材料科学者をサポートする機械学習ソフトウェアの開発などを実現した。これらは、それぞれ CS 課題である耐環境性セラミックス、固体イオニクス材料、触媒材料創製に活用され、大きな成果に繋がった。

### ④ナノ構造をビルトインしたモデル材料創製

ナノ構造情報をもとに具体的な材料創製を進めるためには、ナノ構造をビルトインするための適切なプロセスを選択することが不可欠である。このミッションを効果的・効率的に実行するために、総括班主導で領域内に高圧・高温プロセスセンター (NIMS) と原子層制御プロセスセンター (北大) を構成し、共同・融合研究を実施した。具体的な成果として、高圧合成法によるダイヤモンドと立方晶窒化ホウ素ヘテロ接合界面の形成と発光機能発見、高圧相凍結による新しい酸化チタン光触媒材料の発見、パルスレーザー堆積 (PLD) 法や電界変調法による超精密薄膜合成技術の開発、酸化物二次元系熱電材料の創製などが挙げられる。これらは CS 課題の一環として、ナノ構造デザインに基づく新しい材料創製に繋がる成果となった。

### 研究項目 A03 ナノ構造デザインに基づく新しい材料創製 (計画 3 班, 公募 1 期 5 班, 2 期 6 班)

目標：研究項目 A01 で獲得したナノ構造情報に基づき，A02 において創出されたナノ構造デザイン技術，すなわち情報学的方法論やモデル材料創製技術を活用し，本研究項目において材料創製のエキスパートのもとで各々の CS 課題をターゲットとした新しい材料創製に繋げ，普遍的な材料開発原理を実証する。

#### ⑤ナノ構造デザインに基づく新しい材料創製

##### CS1:機能性セラミックス材料

耐熱合金上に形成した遮熱コーティング材の寿命を支配する酸化アルミニウム膜を高機能化するために，まず研究項目 A01 において，単一モデル界面を用いて STEM 法によりナノ構造情報を獲得した．次に研究項目 A02 において開発したベイズ最適化による高効率の界面構造探索法を適用し，抽出された構造に対して第一原理計算を実施することで，粒界における物質移動を制御するためのナノ構造デザインを施した．これに従って，研究項目 A03 で合成とイオン伝導度評価実験を行ない，設計指針が正しいことを実証した．同様に生体活性の酸化チタンセラミックスについて，表面近傍のナノ構造情報をハイパースペクトルイメージ解析により獲得し，特性向上の合理的な設計指針を得ることに成功した．

##### CS2:固体イオニクス材料

研究項目 A03 において蓄積したリチウム，酸素，プロトン，ヒドリドといった多様な固体イオニクス材料についての巨視的な実験データに立脚し，研究項目 A02 で開発したテンソル分解法による推薦システムを活用して実験計画を立て，A03 において新規物質の合成実験を進めた．また系統的な第一原理計算のよって得られた伝導イオンに関するナノ構造情報を活用し，複雑なイオン伝導メカニズムを解明するための新たなベイズ最適化手法を開発した．その結果，従来比 30 倍の高効率でイオン伝導経路を定量化することに成功した．これらの成果に基づいて，世界で初めてヒドリドイオン伝導性酸水素化物を発見し，電気化学デバイスとして作動することを実証した．またリチウムイオン二次電池の  $\text{LiFePO}_4$  正極については，超長サイクル寿命材料の開発に成功したほか，充放電履歴現象の起源を研究項目 A01 でのハイパースペクトルイメージ解析によって解明し，特性向上の合理的な設計指針を得ることに成功した．

##### CS3:触媒材料

研究項目 A01 で開発した高空間分解能ナノ構造解析実験と第一原理計算により，酸化チタンに担持した金および白金の単原子吸着の安定サイトと，起源となる表面酸素空孔の存在を解明した．得られたナノ構造情報をもとに研究項目 A03 で様々な組み合わせの担持触媒金属でカルボン酸還元反応を行い，触媒活性を機械学習法によってモデル化した．また担持触媒金属における活性序列の予測と最適化モデルの作製に成功した．光触媒に関しては，研究項目 A02 との共同研究により，高压相の結晶構造を凍結させた酸化チタン新材料や，高い活性を示す新物質  $\text{SnMoO}_4$  を発見した．このように，ナノ構造デザインに基づく新材料創製に数多く成功し，設計指針を実証できた．

上述のように，すべての研究項目において，CS 課題の 3 つの材料分野における多様な材料を対象に，ナノ材料科学のフロンティア開拓とナノ構造情報の活用という 2 つのアプローチを密接連携させ，ナノ構造情報を活用した普遍的な材料開発原理を構築するという材料科学の新展開を導くことに成功した．当初計画が 100%以上に達成できただけでなく，様々な新材料創製に成功という期待以上の成果があったと自己評価している。

### 3. 主な研究成果（発明及び特許を含む）

#### 研究項目 A01 ナノ材料科学のフロンティア開拓

##### A01(ア) ナノ構造解析のフロンティア開拓

###### ● 第一原理計算とベイズ最適化による複雑なイオン伝導経路の探索

###### (領域内融合研究, 工学と情報学)

第一原理計算とベイズ最適化を組み合わせることで、高速かつ高精度でポテンシャルエネルギー表面 (PES) を評価する方法論を構築した (図 1)。イオン伝導を支配する領域が結晶全体の一部分であることに着目し、その支配領域のみを選択的に評価する方法である。この PES 評価手法を用いることにより、膨大な多元系材料を高速かつ高精度でスクリーニングでき、CS2 の固体イオニクス材料探索に貢献した。[K. Kanamori *et al.*, Phys. Rev. B 97 (2018) 125124]

###### ● 機能性酸化物表面上の機能元素の局所構造解明

###### (領域内共同研究)

第一原理計算と電子顕微鏡解析実験との密接な共同研究により、ルチル型酸化チタン(110)表面に担持した金および白金の単原子吸着構造と結合状態を解明した (図 2)。長い歴史をもつ酸化チタン表面研究でも、ほとんど注目されなかった底面酸素空孔への吸着メカニズムが重要となることを見出し、CS3 の触媒材料研究に指針を与えた。[K. Matsunaga *et al.* J. Phys. Condens. Matter 28 (2016) 175002]

##### A01(イ) ナノ機能元素解析のフロンティア開拓

###### ● セラミックス粒界の解析・粒界インフォマティクス

###### (領域内融合研究, 工学と情報学)

1 Å 以下の空間分解能を有する走査型透過電子顕微鏡 (STEM) とエネルギー分散型 X 線分光法 (EDS) を併用し、セラミックス粒界の原子構造やそこに濃化する不純物・溶質原子の存在を実空間で直接観察するナノ計測技術を確立した (図 3)。これに機械学習手法を適用することにより、粒界の安定構造を高効率に予測して機能との相関を知る手法、すなわち粒界インフォマティクスという分野を創出した (図 4)。これにより従来は定性的な理解に留まっていたアルミナやジルコニア粒界における溶質偏析挙動を原子レベルで定量的に解明することに成功した。これにより CS1 の機能性セラミックスの高温特性向上の合理的な設計指針が得られた。[B. Feng *et al.* Nature Comm. 7 (2016) 11079, S. Kiyohara *et al.* Sci. Adv. 2(2016) e1600746.]

##### A01(ウ) ナノ電子状態解析のフロンティア開拓

###### ● 非負値テンソル分解法によるハイパースペクトルイメージ解析

###### (領域内融合研究, 工学と情報学)

ナノ構造から得られる STEM-EELS スペクトラムイメージのビッグデータを解析するために、非負値テンソル分解法によるハイパースペクトルイメージ法を開発した (図 5)。これにより、先験的情報なしに構成する小数の特徴量を見出し、ノイズの除去と構成成分スペクトル抽

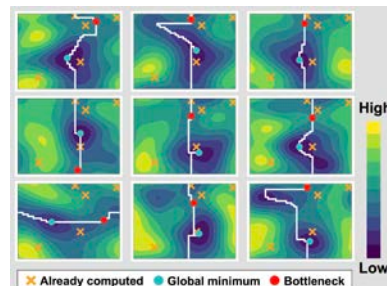


図 1 ベイズ最適化によるイオン伝導経路の探索

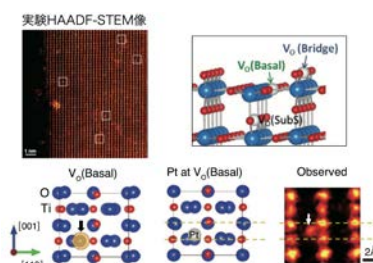


図 2 TiO<sub>2</sub>(110)表面上に吸着した白金単原子の局所構造

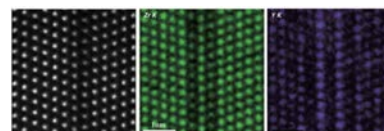


図 3 ジルコニア粒界の STEM 像・EDS マッピング

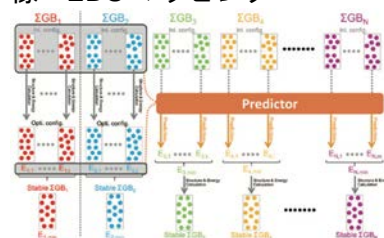


図 4 機械学習による粒界構造予測 (粒界インフォマティクス)

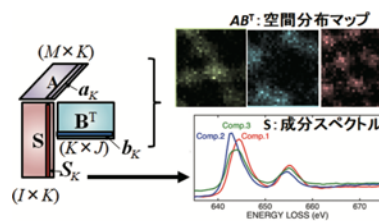


図 5 ハイパースペクトルイメージ解析

出／画像回復や重畳情報の分離とその空間マッピングが可能となった。これを **CS1** の生体活性セラミックスや強磁性体に適用し、従来は実測が困難であった表面や界面近傍の化学結合状態や局所磁気角運動量を定量的に測定することに成功した。 [T. Thersleff, S. Muto *et al.* Sci. Rep. 7 (2017) 44802, J. Rusz, S. Muto *et al.* Nature. Commun. 7 (2016) 12672]

**A01 公募研究 1 期（一杉，高橋，王）（領域内共同研究）**

原子間力顕微鏡複合装置を開発し、ペロブスカイト酸化物最表面における d 電子状態の高分解能測定に成功した（一杉）。ダイヤモンドと立方晶窒化ホウ素の接合界面の原子構造、結合メカニズムを決定した（王）。コヒーレント X 線回折イメージング法によるナノ空間分解能を有する XAFS 法の可能性について検討した（高橋）。

**A01 公募研究 2 期（高橋康，高橋幸，水野）（領域内共同研究）**

MoS<sub>2</sub>/WS<sub>2</sub> ヘテロ接合における水素発生反応活性について走査型電気化学セル顕微鏡による電気化学イメージングを行った（高橋康）。Ce<sub>2</sub>Zr<sub>2</sub>O<sub>x</sub>(CZ)粒子の三次元価数イメージング実験の価数分布像から CZ 粒子内部で価数が不均一に分布している様子を明らかにした（高橋幸）。第一原理計算により、高エントロピー合金における原子空孔の構造と低拡散能の解析を行った（水野）。

**研究項目 A02 ナノ構造情報シンセシスによる機能設計・探索**

**A02(エ) ナノ構造情報に基づいた機能探索**

● 仮想スクリーニング法・推薦システムによる高効率な新物質・新機能の発見（領域内融合研究，工学と情報学）

無機物質データベースをベイズ最適化に基づいて高効率に仮想スクリーニングする方法を開発した（図 6）。この方法に化合物の普遍的特徴量を導入することにより、全無機物質 55,000 件の中から既知の低熱伝導度物質に比べて 1 桁以上熱伝導度が低い物質を効率的に多数見つけ出すことに成功した。これは **CS1** の新しい熱電変換セラミックス材料の開発において、選択肢を大幅に広げるものとなった。また **CS2** の固体イオニクス材料における新物質発見を対象に情報学の問題設定を行い、推薦システムを応用する手法を開拓した。これにより、合成可能性の高い新規化合物の化学組成を提案できた。 [A. Seko *et al.*, Phys. Rev. Mater. 2 (2018) 013805, A. Seko *et al.* Phys. Rev. Lett. 115 (2015) 205901]

● 高圧合成による新規機能性材料の創製（領域内共同研究）

先端電子顕微鏡によるナノ構造解析チーム，第一原理計算チームとの連携のもと，モデル材料において的確なナノ構造を材料にビルトインし，機能発現の基礎を抽出するための物質・材料創製技術として，高圧・高温プロセスを展開した。具体的な成果として，**CS1** での高圧合成法によるダイヤモンドと立方晶窒化ホウ素ヘテロ接合界面の形成と発光機能発現（図 7），**CS3** での高圧相凍結による新しい酸化チタン光触媒材料の発見などが挙げられる。また減圧中の相変化メカニズ

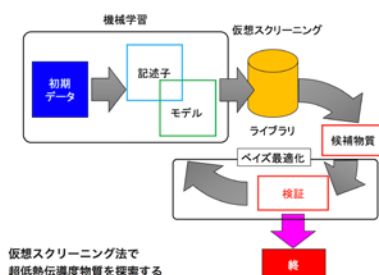


図 6 仮想スクリーニング法

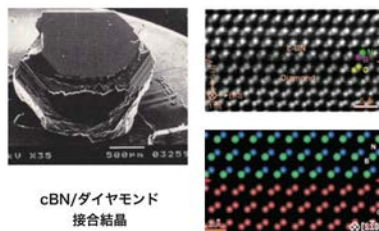


図 7 立方晶窒化ホウ素(cBN)/ダイヤモンド単結晶のヘテロ接合界面

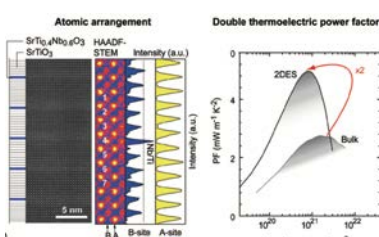


図 8 酸化物二次元電子系熱電材料の創製

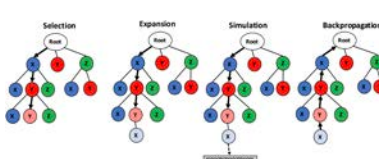


図 9 モンテカルロ木探索

ムに関する研究も進め、高圧相の回収指針の提案を行った。これらの成果は、ナノ構造デザインに基づく新しい材料創製に大きく貢献した。[C.Chen *et al.* Nat. Comm. 6 (2015) 6327]

#### A02(カ) 原子層制御による新しい材料機能探索

##### ● 酸化物二次元電子系熱電材料の創製 (領域内共同研究)

ナノ構造を原子層制御でビルトインするために超精密薄膜合成技術を開発し、領域内共同研究を進めた。CS1として酸化物人工超格子において二次元性を高めることで、熱電特性の大幅な向上を目指した。SrTiO<sub>3</sub>-SrNbO<sub>3</sub>固溶体の熱電特性を実験・計算から調査したうえで、パルスレーザー堆積法により実際に数多くの人工超格子を作製し、バルクの2倍に相当する出力因子を達成した(図8)。これは、二次元性を高めることが熱電材料の高性能化に有効であることを明確に示した初めての結果であり、ナノ構造デザインに基づく新しい材料創製に大きく貢献した。[Y. Zhang *et al.* J. Appl. Phys. 121 (2017)185102]

#### A02(コ) 材料インフォマティクスに適した機械学習法の開拓

##### ● 材料科学者をサポートする機械学習ソフトウェアの開発 (領域内融合研究, 工学と情報学)

物質探索に不可欠なベイズ最適化アルゴリズムのソフトウェア COMBOを開発し、領域内での融合研究に供した。材料研究者が深い専門知識なしに利用できるように、パラメータのチューニングが不要となる工夫を取り入れた。またコンピュータ囲碁で採用されているモンテカルロ木探索(MCTS)プログラムを開発し(図9)、CS1における境界インフォマティクスに活用した。その結果、界面の原子配列を、網羅的探索に比べて100倍以上に高効率に発見することに成功した。これらのソフトウェアは、一般公開され、国際的に領域研究以外にも広く活用されている。[Ueno *et al.* Materials Discovery 4 (2016) 18]

#### A02 公募研究 1期 (永田, 鹿島, 本多, 志賀, 竹内, 池野) (領域内共同研究)

統計熱力学計算のためのデータ駆動型アルゴリズム開発を行った(永田)。マルチタスク学習によるリチウムイオン伝導体の材料探索を行った(鹿島)。線形モデルにより効率良い材料探索が可能であることを示した(本多)。情報学に基づいたスペクトラムイメージ解析法を開発した(志賀)。情報科学手法によるプロトン伝導体におけるエネルギー曲面の評価を行った(竹内)。化学組成の巨大なバラエティのなかからの情報学的手法を用いた酸窒化物蛍光体の材料設計を行った(池野)。

#### A02 公募研究 2期 (Packwood, 本多, 島川, 中平, 池野) (領域内共同研究)

ベイズ最適化による分子配置の効率的予測に成功した(Packwood)。線形モデル上のバンドフィット問題において、最適候補を識別するための特徴量を適切に絞り込み探索するアルゴリズムを構築した(本多)。複合酸化物において異常高原子価 Fe<sup>3.5+</sup>が電荷不均化とサイト間電荷移動の逐次相転移を示すことを解明した(島川)。有機溶媒を用いた水溶液系プロセスで剥離型ナノシート作製法を開発した(中平)。圧縮センシング法を用いたナノ構造からのスペクトル解析法を開発した(池野)。

### 研究項目 A03 ナノ構造デザインに基づく新しい材料創製

#### A03(キ) 耐環境性セラミックス材料のナノ構造制御と材料創製

##### ● 多結晶アルミナの粒界特性を利用した物質移動制御 (領域内融合研究, 工学と情報学)

アルミナ焼結体を用いて酸素ポテンシャル勾配下における膜中の物質移動機構を評価・解析した(図10)。また第一原理計算や電子エネルギー損失分光(EELS)を用いて、粒界構造と物質移動の相関解明に取り組んだ。その結果、多結晶粒界のような整合性の低い粒界では半導体的な特性が増すことと、そのような粒界における電子状態変化が酸素拡散の起源であることを明らかにした。また、高温に曝された膜中の酸素の粒界拡散係数が自己拡散に比べて約1/10に低下すること

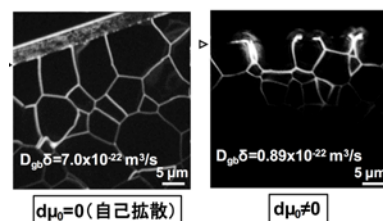


図10 多結晶アルミナ膜の断面表面近傍の酸素トレーサー(<sup>18</sup>O)-SIMSマップ

を発見した。この特性を利用することで、電気伝導特性の大きく異なる酸化物からなる多相積層膜中の物質移動を効果的に制御できることを見出した。[T. Ogawa *et al.* *Acta Mater.* 69 (2014) 365]

### A03(ク) ナノ構造情報に基づいた新しい固体イオニクス材料の創出

#### ● 新しい固体イオニクス材料の創製 (領域内融合研究, 工学と情報学)

純粋にヒドリドイオンだけが固体内を拡散する酸水素化物を発見し、第一原理計算チームとの領域内共同研究によって、イオン伝導機構を解明するとともに、組成を制御することによるイオン導電率の調整に成功した(図11)。また全固体型のデバイスを作製し、ヒドリドイオンを電荷担体とした電気化学デバイスの作動に世界で初めて成功した。さらに本グループで蓄積した実験データをもとに、情報学的問題設定を行い、テンソル分解法による推薦システムを構築し、それに基づいた実験計画により、高効率に新規リチウムイオン固体電解質を探索する手法を開拓した。[G. Kobayashi *et al.* *Science*, 351 (2016) 1314.]

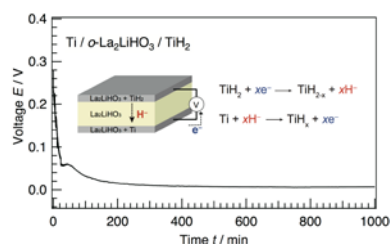


図11 Ti/La-Sr-Li-H-O系電解質/TiH<sub>2</sub>の放電曲線

### A03(ケ) 規整ナノ反応場の構築と新しい触媒機能の創出

#### ● 担持金属触媒における活性秩序の予測と最適化 (領域内融合研究, 工学と情報学)

DFTによる121種類の金属・合金のd-バンド中心のデータに関して、各金属の周期表における族や密度、イオン化エネルギー等の入手可能なパラメータを特徴量とした回帰モデルの構築と機械学習による高速予測を試み、個々の値をすべてDFT計算により求めた場合と比べて、遥かに高速での予測が可能であることを実証した(図12)。本手法を応用することで、理論計算により求めた一部の金属・合金のd-バンド中心の値を用いて、他のさまざまな金属・合金系のd-バンド中心を予測し、活性序列に関する情報や最大活性を示す材料の候補を効率的に見つけることが可能になった。[I. Takigawa *et al.* *RSC Adv.* 6 (2016) 52587.]

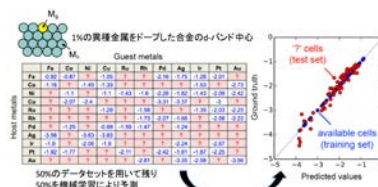


図12 担持金属触媒における活性秩序の予測と最適化

### A03 公募研究1期 (東, 藤田, 横井, 舟窪, 柳田) (領域内共同研究)

ペロブスカイト非鉛圧電材料の設計を行い、高压合成法により単斜晶相を得る事に成功した(東)。希土類複合酸化物等の電子構造、格子振動、磁性および対称性の破れについて明らかにした(藤田)。ゼオライト骨格内原子分布が触媒活性に与える影響を検討した(横井)。HfO<sub>2</sub>基強誘電体を熱膨張率の異なる基板上に作製し、膜の歪が強誘電性に大きな影響を及ぼしていることを確認した(舟窪)。ナノ構造情報に基づき、新しい金属酸化物単結晶ナノワイヤ設計を進めた(柳田)。

### A03 公募研究2期 (舟窪, 北條, 藤井, 山崎, 黒川) (領域内共同研究)

HfO<sub>2</sub>基強誘電相の安定化指針を獲得した(舟窪)。複合酸化物薄膜において強誘電と強磁性ドメインの競合を観察した(北條)。純酸化物イオン伝導体の新物質 SrYbInO<sub>4</sub>を発見した(藤井)。プロトン伝導体ジルコン酸バリウムにおける会合エネルギー決定因子を明らかにした(山崎)。STM観察による3次元アトムプローブ(3DAP)試料の形状と3DAP測定時のイオン検出密度パターンとの相関を見出した(黒川)。

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研究項目 A02 ナノ構造情報シンセシスによる機能設計・探索  
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## 学会発表

1. 中村 篤智, 機械・電機・光のマルチフィジックス欠陥制御の新展開, 第65回応用物理学会春季学術講演会, 2018年3月(招待講演)
2. 松永 克志, 貴金属/TiO<sub>2</sub> 界面における結合状態と点欠陥形成, 日本金属学会 2017 年秋期(第161回)講演大会, 2017年9月(基調講演)
3. 松永 克志, セラミックスのナノ構造と特性に関する理論解析, 日本セラミックス協会 2017 年会, 2017年3月(平成28年度学術賞受賞講演)

4. 松永 克志, セラミックス系材料における塑性変形・破壊のナノ構造計算解析, 日本金属学会 2015 年秋期 (第 157 回) 講演大会, 2015 年 9 月 (基調講演)
5. 中村 篤智, 酸化物双結晶を用いた転位の構造解析と物性評価, 日本金属学会 2015 年秋期 (第 157 回) 講演大会, 2015 年 9 月 (基調講演)
6. N. Shibata, "Atom-resolved differential phase contrast scanning transmission electron microscopy", IAMNano 2017, Singapore, November 14, 2017, Invited.
7. T. Mizoguchi, "Materials Informatics for Nanostructures", The Association of East Asian Research Universities (AEARU) Advanced Materials Science Workshop 2017, Invited.
8. R. Ishikawa, "Direct Observation of Functional Point Defect Structures in Nitrides", 8<sup>th</sup> International Workshop on Spinel Nitrides and Related material, Rudesheim, Germany, September 8, 2016, invited.
9. E. Tochigi, A. Nakamura, T. Mizoguchi, N. Shibata, Y. Ikuhara, "TEM study of dislocations and stacking faults in low-angle grain boundaries of alumina", THERMEC2016, Graz, Austria, May 31, 2016, invited.
10. R. Ishikawa, A.R. Lupini, S.D. Findlay, T. Taniguchi, S.J. Pennycook, "Quantitative Electron Microscopy and the Application by single Electron Signals", Microscopy and Microanalysis 2015, Portland, OR< USA, August 5, 2015, invited
11. T. Mizoguchi, "Theoretical ELNES: Excitonic and Vibrational calculations", Frontier of electron microscopy for materials science for materials science (FEMMS) 2015, Lake Tahoe, CA, USA, September 18, 2015, invited.
12. N. Shibata, "Development of an advanced scanning transmission electron microscope for material science research", Millennium Science Forum Sir Martin Wood prize Lecture, Glasgow, UK, June 23, 2014, invited.
13. N. Shibata, S.D. Findlay and Y. Ikuhara, "Interface characterization by advanced STEM", Frontiers of Electron Microscopy in Materials Science 2013, Lorne, VIC, Australia, September 11, 2013, invited.
14. T. Mizoguchi, "Identification and characterization of defects in functional materials: first principles calculation and STEM-EELS", PACRIM-8, Waikoloa, Hawaii, USA, August 8, 2013, invited.
15. 武藤 俊介, "構造化データ融合法によるテンソル分會を適用したハイパー顕微分光データからの情報抽出", 日本顕微鏡学会超高分解能顕微鏡法分科会, マホロバ・マインズ三浦, 神奈川, February 23-24, 2018
16. S. Muto, "In situ observation of catalytic reactions under gas atmosphere by reaction science high-voltage scanning transmission electron microscope equipped with quadrupole mass spectrometer, "The 3<sup>rd</sup> East-Asia Microscopy Conference (EAMC3), Busan, Korea, November 7-10, 2017
17. 武藤 俊介, "ナノ電子顕微分光への情報処理技法の応用", 第 46 回薄膜・表面物理基礎講座 2017, 名古屋大学 VBL ホール, 愛知, November 17, 2017
18. 武藤 俊介, "ハイパー分光スペクトルイメージングデータによる化学イメージング情報統計学によるエータ処理を正しく使うために-", 第 7 回 CSJ 化学フェスタ 2017, タワーホール船越, 東京, October 17-19, 2017
19. 武藤 俊介, "情報統計処理による信号抽出法の基礎", 第 33 回分析電子顕微鏡討論会, 幕張メッセ国際会議場, 千葉, September 5-6, 2017
20. S. Muto, "Signal mining for chemical imaging from hyperspectral image data, 3<sup>rd</sup> International Workshop on TEM Spectroscopy in Materials Science", Uppsala, Sweden, June 19-22, 2017
21. S. Muto, "Hyperspectral Image Analysis of Spatially/Spectrally Overlapped Datasets for Chemical Imaging", The 19<sup>th</sup> Scientific International Symposium on SIMS and Related Techniques Based on Ion-Solid Interactions, SISS19, Miraka Messed, Kyoto, May 11-12, 2017
22. S. Muto, "Multi-Way Hyperspectral Image Analysis Based on Scanning Transmission Electron Microscopy and Associated Spectroscopic Methods", 2017 MRS Spring Meeting & Exhibit, Phoenix, Arizona, USA, April 17-21, 2017

23. 武藤 俊介, “ビッグデータ時代の微細構造解析支援ートップサイエンスと実材料分析ー”, 共用・計測合同シンポジウム 2017 先端計測研究と共用推進による材料イノベーション, 物質・材料研究機構, March 9, 2017 (基調講演)
24. 武藤 俊介, “新しい情報・統計理論に基づくスペクトル分解ー化学イメージング法の開発”, Spring-8 材料構造の解析に役立つ計算科学研究会 (第 3 回) / 第 10 回 Spring-8 先端利用技術ワークショップ, (株)ニチイ学館神戸ポートアイランドセンター, February 27, 2017
25. 武藤 俊介, “ナノ電子顕微分光への情報処理技法の応用”, 「先端計測インフォマティクス 大量データ時代の情報活用」ワークショップ, 物質・材料研究機構, January 19, 2017
26. 武藤 俊介, “複合電子顕微分光と情報統計処理による機能元素/物性定量分析ーTwo-way から Multi-way 解析へ, ナノ材料から宇宙へー”, 日本金属学会 2016 年秋期 (第 159 回) 講演大会, 大阪大学豊中キャンパス, September 21-23, 2016 (基調講演)
27. 武藤 俊介, “ナノ電子分光への情報処理技法の応用”, 第二回元素プロジェクト<研究拠点形成型>/大型研究施設連携シンポジウム「局所構造制御で物質から材料へ」, 東京大学伊藤国際学術研究センター, January 22, 2016
28. S. Muto, “Mind the Noise: Mining Hidden Information from Spectroscopic Datasets”, オングストローム研究所ランチセミナー, ウプサラ大学, December 15, 2015
29. S. Muto, J. Ruzs, K. Tatsumi, T. Thersleff, K. Leiffer, “Current progress in nanometric magnetic moment measurements based on electron magnetic circular dichroism”, Magnetics and Optics Research International Symposium 2015 (MORIS2015)m TUT-USM Penang, Penang, Malaysia, Nov. 29-December 2, 2015
30. S. Muto, M. Shiga, K. Tatsumi, K. Tsuda, “Current progress in data mining technique applying to digital spectral image datasets”, ALC'15, Kunibiki Messe, Matsue, Shimane, October 25-30, 2015
31. S. Muto, “Mind the Noise: Mining Hidden Information from Spectroscopic datasets”, NIMS Conference 2015, Tsukuba International Congress Center, July 14-16, 2015
32. S. Muto, “Application of EDX Spectroscopy”, The 2<sup>nd</sup> Uppsala TEM spectroscopy workshop, オングストローム研究所, ウプサラ大学, May 18-20, 2015
33. S. Muto, “Quantitative element/site-selective microanalysis using high-angular resolution electron channeled X-ray/electron spectroscopy”, The 3<sup>rd</sup> Croatian Microscopy Congress (HMK2015)m the Hotel Adriana, April 26-19, 2015
34. 武藤 俊介, “エネルギー関連機能材料のナノオーダー解析ー電池・触媒の STEM 分光マッピングを中心にー”, 2014JEOL 先端材料解析ソリューションセミナー, グランドティアラ名古屋駅前, November 14, 2014
35. 武藤 俊介, “電子磁気円二色性に基づくナノ領域磁気角運動量定量測定”, 第 30 回分析電顕討論会, 幕張メッセ国際会議場, September 2-3, 2014
36. S. Muto, K. Tatsumi, M. Ohtsuka, “Element/site-selective microanalysis using high-angular resolution electron channeled x-ray/electron/light spectroscopy”, The 4<sup>th</sup> International Symposium on Advanced Microscopy and Theoretical Calculations (AMTC4), アクトシティ浜松コンgresセンター, My 8-10, 2014
37. 武藤 俊介, “Recent development of EMCD technique:toward spin nanoscopy using STEM-EELS”, 第 13 回 ESICMM セミナー, 独立行政法人物質・材料研究機構, April 16, 2014
38. I. Tanaka, Materials Discovery Through Machine Learning Process, 9<sup>th</sup> International Symposium on Nitrides, 2017, invited
39. H. Hayashi, DFT-Based Screening of novel Sn(II)-Based oxide Photocatalysts, 10<sup>th</sup> International Conference on the Science and Technology for Advanced Ceramics. 2017
40. 田中 功, 第一原理計算とインフォマティクス手法を用いた材料, 日本金属学会 2017 年秋期講演大会, 2017, invited

41. 世古 敦人, 行列およびテンソル分解を用いた新規無機化合物の推薦氏鶴テム, 日本金属学会 2017 年秋期講演大会, 2017
42. 林 博之, 無機化合物データベースの機械学習に基づいた新規 Li 複合, 日本金属学会 2017 年秋期講演大会, 2017
43. I. Tanaka, Real and virtual screening for materials discovery through first principles calculations, Workshop I: Machine Learning Meets Many-Particle Problems, 2016 invited.
44. I. Tanaka, Thermal conductivity of spinel nitrides and related materials by first principles calculations, 8<sup>th</sup> Intl. Workshop on Spinel Nitrides and Related Materials, 2016, invited.
45. Y. Hinuma, Y. Kumagai, H. Hayashi, F. Oba and I. Tanaka, Calculating binary oxide surface properties with a high-throughput procedure, MRS Fall Meeting, 2016
46. I. Tanaka, Accelerated Discovery of Ceramic Materials via Systematic Density-Functional Calculations, 11<sup>th</sup> Intl. Conference on Ceramic Materials and Components for Energy and Environmental Applications, 2015, invited.
47. I. Tanaka, Materials Genome and materials design, 第 1 回マテリアルズ・ゲノム (情報統合型物質・材料研究に関する日米ワークショップ), 2015, invited.
48. I. Tanaka, Efficient materials Exploration based on Systematic Density-Functional Calculations and Machine Learning Techniques, AMTC4, 2014, invited.
49. T. Taniguchi, "High pressure synthesis of cubic and hexagonal boron nitride single crystals and their impurity control", International Workshop UV Mater & Devices 2017 (IWUMD2017), November 14, 2017, invited.
50. 谷口 尚, "高圧・高温プロセスによる窒化物系高密度相の機能探索", 日本金属学会 2017 年秋期大会, 札幌, September 6, 2017, invited.
51. T. Taniguchi, "Synthesis hexagonal Boron High pressure synthesis of polymorphic phase of Boron Nitride", MRS spring meeting, April 17, 2017, invited
52. T. Taniguchi, "Synthesis of high purity hBN and other 2D single crystals", Graphene week, June 13, 2016, invited.
53. T. Taniguchi, "High pressure synthesis of boron nitride polymorphic phases and their applications", Thermec 2016, May 30, 2016, invited.
54. 谷口 尚, "ダイヤモンド, cBN 等の硬質材料・ワイドギャップ材料の高圧合成・不純物制御", 日本材料学会 学術講演会, may 23, 2015
55. T. Taniguchi, "Impurity control in high pressure synthesis; Realization of promising potentials of superhard material of cubic boron nitride", 1<sup>st</sup> Intl. forum on the Advanced Materials Processing, Kumamoto University, March 6, 2015, Invited
56. 谷口 尚, "高圧・高温プロセスを李王した窒化物系高密度相合成と新機能探索", 日本金属学会 2014 年秋期大会, 名古屋, September 24-26, 2014, invited.
57. T. Taniguchi, "Impurity control of 2D-/3D- Boron Nitride crystals and their functionalization", ISNT2014, August 31, 2014, invited.
58. T. Taniguchi, "High pressure synthesis of BN and BCN crystals and their functionalization", IUCR2014, August 5, 2014, invited.
59. H. Ohta, Electrochemical function modulation of oxides using three-terminal thin film transistor structure with water infiltrated insulate, The 3<sup>rd</sup> Functional Oxide Thin Films for Advanced Energy and Information Technology, Roma, Italy, July 5-8, 2017
60. H. Ohta, Electric field modulation of thermopower in two-dimensional electron gas, IUMRS-ICAM 2017, Kyoto, August 27-September 1, 2017
61. 太田 裕道, 固相エピタキシャル成長法を駆使した機能性酸化物ナノ層の創製, 日本金属学会 2017 年秋期講演大会, 北海道, September 6-8, 2017
62. H. Ohta and Y. Zhang, Double enhancement of thermoelectric power factor in oxide two-dimensional electron system via precise dimensionality control, 2017 Fall KPS Meeting, Gyeongju, Korea, October 25-27, 2017
63. T. Katase and H. Ohta, Room-temperature-protonation-driven optoelectronic device with water-gated thin-film-transistor structure, the 8<sup>th</sup> Intl. Conference and Exhibition on Lasers, Optic & Photonics, Las Vegas, USA, November 15-17, 2017

64. H. Ohta and A. Sanchela, Thermopower of oxide heterostructure, ICAMD2017, Jeju, Korea, December 5-8, 2017
65. H. Hiramatsu and H. Hosono, Heteroepitaxial growth, critical current, and electric field-induced phase transition of iron-based layered selenides/pnictides, IUMRS-ICAM, Kyoto, August 27-, September 1, 2017
66. H. Hiramatsu and H. Hosono, Electronic Phase Transition at Interface between Solid and Ionic Liquid under Gate Voltage, MRS Fall Meeting 2017, Boston, USA, November 26-December 1, 2017
67. 太田 裕道, 導電性酸化物薄膜の物性改質方法, 第 64 回応用物理学会春季学術講演会, パシフィコ横浜, 神奈川, March 14-17, 2017
68. H. Ohta and W.S. Choi, Unusually large Thermopower of nanostructured oxides, ENGE 2016, Jeju, Korea, November 6-9, 2016
69. 太田 裕道, 金木奨太, 橋詰 保, 熱電能電界変調法 : AlGaN/GaN-MOSHEMT, 2016 年第 77 回応用物理学会秋季学術講演会, 朱鷺メッセ, 新潟, September 13-16, 2016
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71. H. Ohta and T. Katase, Water electrolysis induced modification of functional oxides-Thermoelectric properties-, IUMRS-ICAM 2015, Jeju, Korea, October 25-29, 2015
72. 太田裕道, 水の電気分解を利用した機能性酸化物ナノ層創製, 日本金属学会 2015 年秋季講演大会, 福岡, September 16-18, 2015
73. M. Shiga and S. Muto, Automatic Spectral Imaging Analysis Based on Machine Learning, The 8<sup>th</sup> Intl. Workshop on Electron Energy Loss Spectroscopy and Related Techniques(EDGE2017: Enhanced Data Generated by Electrons), 2017
74. S. Kitaoka, Mass-transfer in EBC materials under oxygen potential gradients at high temperatures, Winter Study Group on High Performance Materials, CA, USA, 2018
75. H. Moriwake et al., Mechanism of polarization switching in wurtzite-structured zinc oxide films, Fundamental physics of ferroelectrics 2017, Williamsburg, USA, 2017
76. A. Kuwabara et al., First principles calculations of defect clustering in acceptor-doped BaZrO<sub>3</sub>, Nonstoichiometric compounds VI, Santa Fe, USA, 2016
77. S. Kitaoka et al., Mass-transfer in Polycrystalline Alpha-Alumina under Oxygen Potential Gradients at High Temperatures: An Experimental Approach, The Intl. Symposium of High-temperature Oxidation and Corrosion 2014, Hakodate, 2014
78. 菅野了次, 超イオン導電体の創出と全固体電池の開発, 日本化学会第 98 春季年会, 2018
79. R. Kanno, All-solid-state battery-Developments of Materials and Devices, Intl. Battery Association, 2018
80. 小林玄器, Ba-Li 系酸水素化物の合成と H-導電特世知, 第 58 回高圧討論会, 名古屋大学, 2017
81. R. Kanno, Developments of New Ionic Conductors and Their Application to All -Solid-State Batteries, 232<sup>nd</sup> ECS Meeting, Maryland, USA, 2017
82. I. Muhammad, Synthesis and lithium-ion conductivity of LiSr-B<sub>2</sub>O<sub>6</sub>F (B=Nb<sup>5+</sup>, Ta<sup>5+</sup>) with pyrochlore structure, 電気化学会第 84 回大会, 2017
83. G. Kobayashi, Synthesis and H-Conductivity of Ba<sub>2</sub>LiH<sub>3</sub>-2xO<sub>1+x</sub>,]
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86. 小林玄器, ヒドリド導電性酸水素化物の合成, 粉体粉末冶金協会平成 27 年度春季大会, 2015
87. K. Suzuki, Analysis of Coating Effects on LiMn<sub>2</sub>O<sub>4</sub> Epitaxial Thin Film Electrode, LiBD2015 (Lithium Battery Discussions)-Electrode Materials, 2015
88. 小林玄器, 新規酸水素化物 Ba<sub>2</sub>LiH<sub>3</sub>O H-の導電特性, 第 41 回固体イオニクス討論会, 2015
89. R. Kanno, In situ X-ray and Neutron Scattering Studies on Electrode-electrolyte Interface in



- Lithium Battery, 65<sup>th</sup> Annual Meeting of the International Society of Electrochemistry, 2014
90. M. Hirayama, New Analytical Tool for Electrochemical Interfaces- in Situ Neutron Reflectometry, the 17<sup>th</sup> Intl. Meeting on Lithium Batteries (IMLB 2014), 2014
  91. 小林玄器, K<sub>2</sub>NiF<sub>4</sub> 型構造の新規酸水素化物におけるヒドリド導電特性, 第 41 回固体イオニクス討論会, 2013
  92. S. Takakusagi and K. Asakura, PTRF-XAFS Study of Single Metal Dispersion on an Oxide Single Crystal Surface by Premodification with a Functional Organic Molecule, Intl. Congress on Pure & Applied Chemistry (ICPAC) 2018, Cambodia, March 8, 2018, invited.
  93. K. Hara, Catalysis with high density molecular monolayers for organic transformation, European Organic Chemistry Congress, Amsterdam, Netherlands, March 3, 2017, invited.
  94. K. Shimizu, Cooperative catalysis of Lewis acid and Pt cluster for hydrogenation of carboxylic acids, amides and Co<sub>2</sub>, I2CNER Intl. Workshop 2016, Fukuoka, February 4, 2016,

## 図書

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3. 溝口照康, 一般社団法人 日本原子力学会, アクチノイド物性研究のための計算科学入門 第 3 章「第一原理計算の応用」2013, 230
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## 5. 産業財産権

### 出願

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2. 名称：高感度昇温脱離ガス分析装置, 発明者：細野秀雄, 半那拓, 平松秀典, 番号:特願 2017-034677, 出願年月日：2017 年 2 月 27 日, 国内外の別:国内
3. 名称：半導体装置, 発明者：太田裕道, 片瀬貴義, 鈴木雄喜, 番号：JP2016/050206, 出願年月日：2016 年 1 月 6 日, 国内外の別：PCT
4. 名称：膜及びそれを備える積層物, 発明者：松平恒昭, 北岡諭, 小川貴史, 柴田直哉, 幾原祐一, 権利者：同上, 番号：特願 2016-42718, 出願年月日:平成 28 年 3 月 4 日, 国内外の別：国内