寄附講座　硬質材料環境調和設計学講座
Endowed Division / Course for Environmental harmony design of hard materials

超硬合金等の硬質材料について最高特性発現と環境調和性の設計学（シミュレーション）構築を目指す

Development of designing (simulation) study for maximum properties and environmental harmony in cemented carbide and other hard materials

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当研究分野では、切削工具、耐摩耗工具に用いられる炭化タングステン - コバルト（WC-Co）超硬合金などの硬質材料において環境資源問題と材料特性等を調和させること（環境調和設計）を目的とした研究開発を進めている。新規硬質材料の基礎研究、シミュレーション、材料設計データベースの構築等を行う。メカニズム解明などの基礎研究の成果が実用的な観点からどのような意味をもつかを明らかにする。硬質材料における資源問題の解決策（希少金属の低減・代替技術など）の基礎研究を行い、硬質材料における資源問題や環境問題を解決する材料設計技術開発を目指す。

We are conducting research and development aimed at harmonizing environmental resource issues and material properties (environmental harmony design) with hard materials, such as tungsten carbide-cobalt (WC-Co) cemented carbides, used for cutting tools and wear-resistant tools. Basic research on new hard materials, simulation, and the construction of a material design database will be conducted. We will clarify the meaning of the basic research results, such as mechanism elucidation, from a practical standpoint and conduct basic research on solutions to resource problems in hard materials (e.g., technologies to reduce and substitute rare metals), aiming to develop material design technologies to solve resource and environmental problems in hard materials.

超硬合金材料の基礎研究

超硬合金材料では近年、従来よりも極めて高い強度が得られる超微粒超硬合金が新規材料として開発され、その基礎研究が重要となっている。また、超硬合金の工業製品においては形状品質や希少金属（W，Co 等）の低減･代替技術の研究なども重要な課題である。本研究室ではこれらの課題に関する研究を企業と連携して行っており、最近では超硬合金の強度と欠陥の関係、超硬合金の焼結時における液相移動と変形、超硬合金の Co 代替材料に関する研究を進めている。

材料プロセスと組織形成のシミュレーション

硬質材料の多くは粉末成形～焼結プロセスによって作製されるが、各プロセスにおける因子は非常に多く、また組織への影響は極めて複雑であるため、シミュレーションの活用が有効である。本研究では、モンテカルロ法、有限要素法、離散要素法などを用いて、硬質材料の材料プロセスにおける組織形成と変形のシミュレーション研究を行っている。樹脂を含んだ粉末成形の離散要素法シミュレーションの計算因子と組織、成形圧力の関係についての検討や、超硬合金を対象とした液相焼結・粒成長の組織形成シミュレーション、粉末金型成形と焼結を連続させたプロセスのシミュレーション、基板拘束された焼結における組織変化と変形の連携シミュレーションの開発を行っている。

硬質材料の特性のシミュレーション

本研究では、硬質材料の機械的特性のシミュレーションを有限要素法と離散要素法を用いて行っている。最近では、超硬合金中の欠陥サイズ、欠陥の分布、欠陥の強度が超硬合金の強度と破壊挙動に与える影響について、離散要素法を用いたシミュレーション研究を行っている。

材料設計データベースの構築

各種のシミュレーションや計算状態図の結果を集積し、材料設計データベースとしての構築を行う。WC と種々の結合相（Co、Ni 等）および各種添加物（TiC、VC 等）の状態図計算、液相焼結・粒成長シミュレーションにおける各因子と組織（粒径、気孔率等）の結果をまとめ、データベース化を進めている。また、既報の組成、プロセスと機械的特性の関係に対して機械学習の適用を進めている。

学会等での活動

川上優：粉体粉末冶金協会理事、同協会硬質材料委員会委員長、同協会粉体および粉末冶金出版編集委員、塑性加工学会代議員等

寺坂宗太：粉体粉末冶金協会代議員

Basic research on cemented carbide materials

Ultra-fine-grained cemented carbides with extremely higher strength than before have been developed as new materials in recent years, and basic research on these materials has become important. In addition, research on shape quality, rare metal reduction (W, Co, etc.), and alternative technologies are also important issues for industrial cemented carbide products. Our laboratory has been conducting research on these issues in cooperation with companies. Recently, we have been studying the relationship between strength and defects in cemented carbides, liquid-phase migration and deformation during sintering of cemented carbides, and Co substitute materials for cemented carbides.

Simulation of material processes and microstructure development

Most hard materials are fabricated by the powder compaction to sintering process. Because there are so many factors in each process and their effects on the microstructure are extremely complex, the use of simulation is effective. In this study, we are conducting a simulation study of microstructure development and deformation in the material process of hard materials using the Monte Carlo method, finite element method, and discrete element method. We are investigating the relationship between the calculation factors and the structure/compacting pressure in discrete element method simulations of compacting powder containing resin, as well as developing (1) simulations of liquid-phase sintering for cemented carbides, (2) simulations of continuous processes of powder compaction and sintering and (3) a coupling simulation of microstructural changes and deformation due to substrate constrained sintering.

Simulation of hard material property

The mechanical properties of hard materials are simulated using the finite element method and the discrete element method. Recently, we have been conducting simulation research using the discrete element method to investigate the effects of defect size, defect distribution, and defect strength in the cemented carbide on the strength and fracture behavior of the cemented carbide.

Construction of material design database

We are constructing a materials design database by accumulating the results of various simulations and phase diagram calculations. We are compiling phase diagram calculations of WC and various binder phases and additives, and the various factors and structures in the liquid-phase sintering simulation and creating a database. We are also working on applying machine learning to the relationships between previously reported compositions, processes, and mechanical properties.

Activities in academic societies

Masaru Kawakami:
Director of Japan Society of Powder and Powder Metallurgy, Chairperson of Technical Division of Hard Materials Committee of Japan Society of Powder and Powder Metallurgy, Publication Editorial Committee of the *Journal of the Japan Society of Powder and Powder Metallurgy*, Representative of the Japan Society for Technology of Plasticity, etc.

Sota Terasaka:
Representative of Japan Society of Powder and Powder Metallurgy

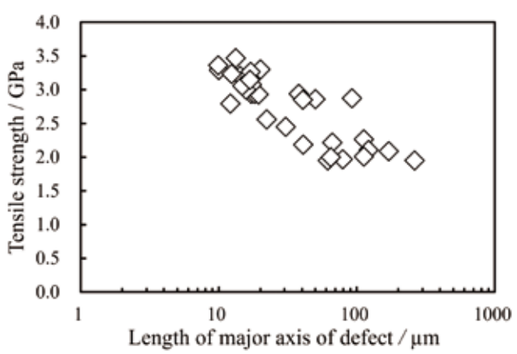

Fig. 1 Relationship between tensile strength and the length of major axis of defect of ultrafine-grained cemented carbides.

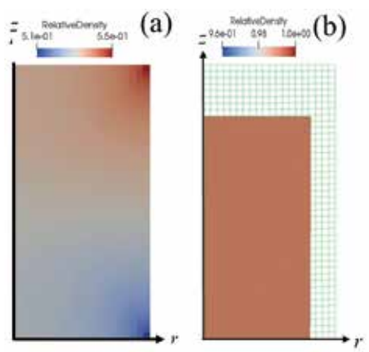

Fig. 2 Simulation results of continuous powder compaction and sintering processes. (a) density distribution of green compact, (b) shrinkage and shape of sintered body.

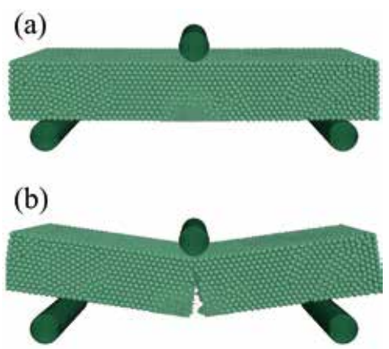

Fig. 3 3D simulation of the strength of cemented carbide using discrete element method. (a) before destruction, (b) after destruction.

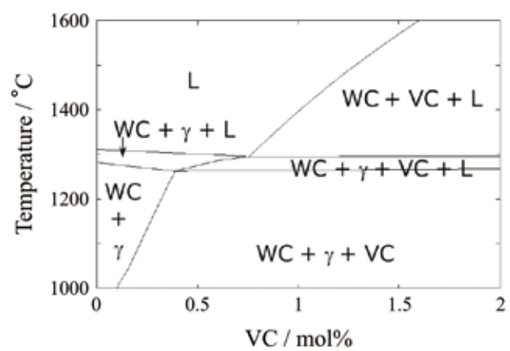

Fig. 4 VC-$W_{0.45}C_{0.45}Co_{0.1}$ pseudo-binary calculation phase diagram.