プロセス・インフォマティクスを用いた排ガス浄化用合金触媒の高効率材料探索

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Efficient Materials Discovery for Exhaust Gas Purification Alloy Catalysts Using Process Informatics ([1]*Honda R&D Co., Ltd*) ○Hitoshi Mikami,[1] Hiroto Tsuchiya,[1] Azusa Kamiyama,[1] Masafumi Sakota,[1]

High-entropy alloys (HEAs) consisting of five or more constituent elements have been applied to catalysts, and multi-element nano-alloy catalysts with specific reactivity and durability have been reported. HEAs, unlike conventional alloys, is characterized by incorporating a diverse array of elements. This alloy not only constitutes isoatomic fraction solid solution alloys but also encompasses compositionally complex alloys with non-uniform element ratios, alloys containing multiple principal elements, and precipitates with non-uniform ratios. Consequently, there exists the potential for the emergence of a novel alloy system that deviates from traditional alloy frameworks, offering anticipated superior properties.

In the discovery for HEAs catalysts, there is a huge search space for element and composition selection and optimization of synthetic conditions. In addition, alloy catalysts have alloy-specific degradation issues such as alloy separation and degradation of support materials due to separated elements, making it difficult to screen only by digital space and initial activity.

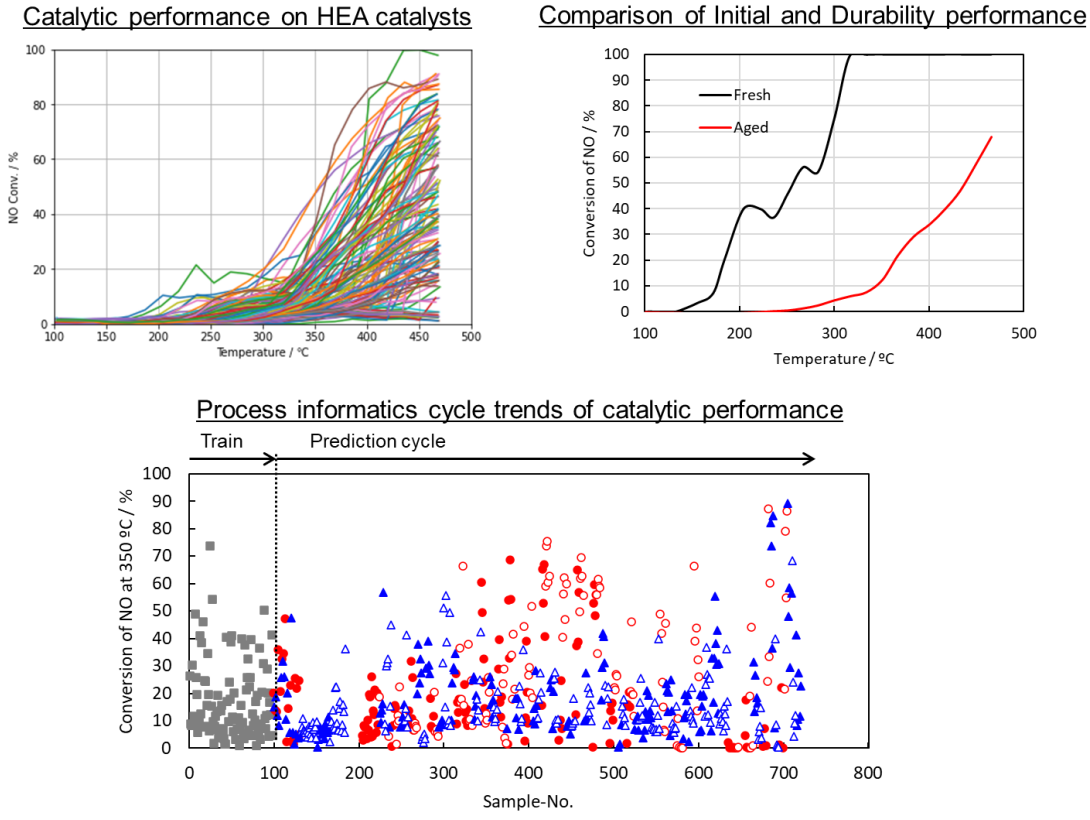
We have developed a high-throughput screening evaluation system with the ability to evaluate purification performance in consideration of durability and to collect, store, and analyze large amounts of data, coupled with efficient exploration of elements, compositions, and synthetic conditions using process informatics. This article introduces effective automotive exhaust gas purification catalysts for low-temperature activity and low cost, as well as practical applications and future developments.

Keywords：high-throughput screening, initial degradation, Automotive catalyst, multi-element nano-alloy

排ガス浄化用 2 元合金触媒の効率的な探索として，触媒合成，活性評価による実験的スクリーニングと TEM 観察，分光分析などによるメカニズム解明や計算化学とデータ科学によるデジタルスクリーニングに取り組んできた [1-2]。近年，５種類以上の構成元素からなるハイエントロピー合金（HEAs）による高機能化を触媒に応用し，特異的な反応性や耐久性を有す多元素ナノ合金触媒が報告されている [3]。HEAs は，等原子分率固溶体合金だけでなく，Compositionally Complex Alloy や Multi Principal Element Alloy といった等原子分率から外れた高濃度固溶体合金や析出物を含めると，これまで探索されなかった多元系状態図の中央近傍領域の化学組成をもつ新規な合金であり，優れた特性を示す未踏の合金系創出の可能性を有す。一方，HEAs 触媒探索は，5 種類の元素，組成選択だけで 10^{98} 通りを超え，かつ合成条件を含めると最適

化には膨大な空間を探索する必要がある。また，合金触媒は，合金分離や分離元素によるサポート材劣化など合金特有の劣化課題を有すため，デジタル空間や初期活性のみでスクリーニングすることは困難である。

耐久性を考慮した NOx，CO，HC 成分の浄化性能評価を実行する機能や大量サンプルの取り扱い，データ収集，格納，解析の自動化機能を備えたハイスループットスクリーニング評価システムと元素，組成および合成条件を効率的に探索するプロセス・インフォマティクスを融合し，自動車排ガス浄化触媒の課題である浄化性能の向上と貴金属使用コスト低減を解決する材料探索の実践的応用した取組み詳細と今後の展望について紹介する。



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