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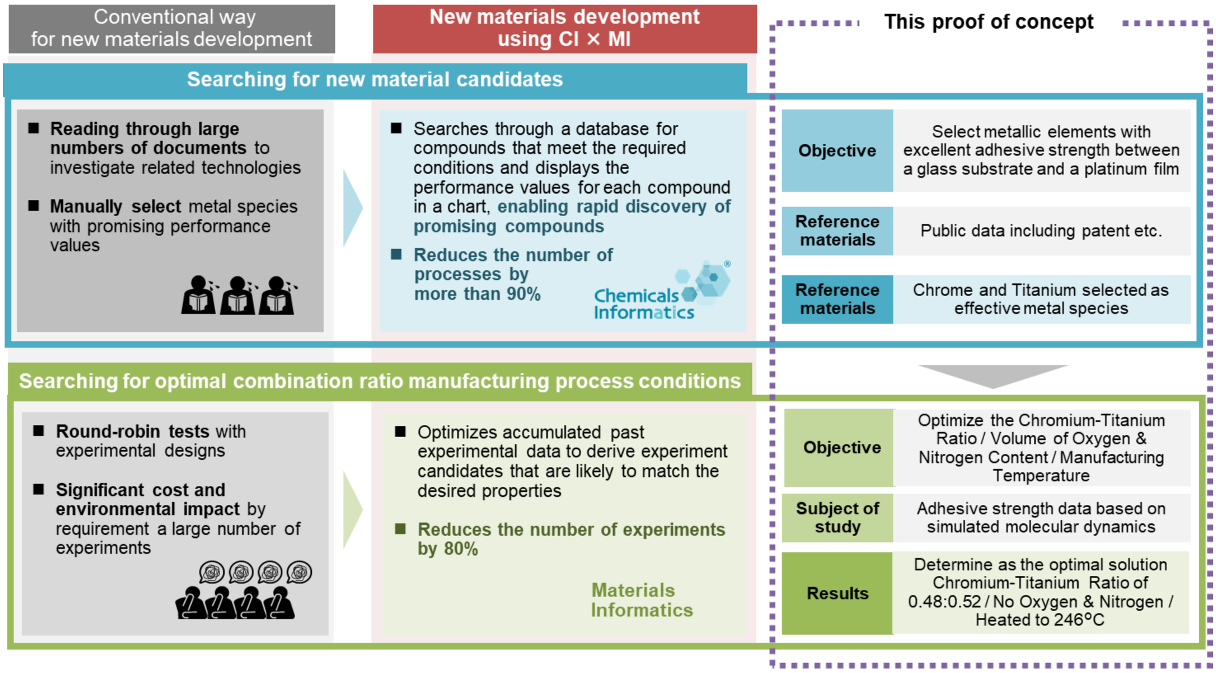
Contributing to Efficient Development of Metal Thin Film Materials by Using Chemicals Informatics and Materials Informatics



Outline Figure

Tokyo, February 8th, 2024 – Hitachi High-Tech Corporation ("Hitachi High-Tech") has conducted a proof of concept ("PoC") trial using Chemicals Informatics ("CI") and Materials Informatics ("MI") to improve the efficiency of developing metal thin film materials used in electronic and other devices. The PoC demonstrated an overall workload reduction more than 80% even when developing new materials, showing that these tools can be used to streamline operations.

In recent years, MI—which utilizes AI to derive optimal combination ratio and composition of materials based on accumulated past experimental data—has been increasingly used to reduce the amount of trial-and-error during the development of materials. CI is a Hitachi High-Tech's proprietary service that uses AI to analyze public data such as patents and select optimal materials for development. CI and MI contribute to the efficiency of development.

The PoC clarified that even new materials with no accumulated past experimental data can be developed more efficiently by combining Hitachi High-Tech's MI with CI. This eliminates the document research and round-robin test with experimental designs*1, thereby improving the efficiency of developing new materials.

Hitachi High-Tech intends to offer the process of this PoC as a service for customers primarily at chemical and material manufacturers, whose demand for increasingly sophisticated and efficient development processes is escalating. The service will not only improve the efficiency of development but also help to mitigate environmental impact by reducing the amount of experimentation required during the development process.

*1 Experimental designs : A method of conducting experiments under a combination of conditions, using a combination of conditions to derive the necessary experiments without omission through statistics, and analyzing the results.

Background of the PoC

The demand for highly sophisticated materials is greater than ever, not only for their functionality but also for how they can be used to solve social issues such as achieving a carbon-neutral/decarbonized society. There is a rising need for DX (Digital Transformation) and GX (Green Transformation) in order to fundamentally strengthen R&D and improve operational efficiency, so many organizations have actively introduced MI as an AI-enhanced method of developing new materials. MI is useful in fields where existing materials have already been developed, but it cannot be used to improve efficiency when developing new materials, where there is no prior accumulated data to pull from during the selection of raw materials. As such, a new tool was needed.

Details of the PoC

This PoC tested the development of metal thin film materials that are used in electronics and other devices.
Metal thin films are created by depositing atoms onto substrates made from materials such as silicon or glass to form thin film layers, which are laminated and used to make electronic devices. A weak bond between the substrate and the metal thin film can cause the film to peel away, resulting in poor performance, so strong adhesion is a key design consideration, but design of adhesion need many development process. The PoC demonstrated a reduction of more than 80% in the number of development processes compared to conventional methods by using CI to determine the most suitable metallic elements for the adhesion layers between substrates and metal thin films, and using MI to determine the best combination ratios of metallic elements and the optimal conditions for manufacturing process.

1. Using CI to select optimal materials based on patent data

Previously, selecting the ideal materials for development involved reading through extensive reference documentation to find the necessary information, then conducting round-robin tests with experimental designs for all of the candidate materials to verify which one works best.
In this PoC, we discovered the optimal material for a strong adhesive layer between a glass substrate and a platinum film by using CI. As information required for CI, we input 2 kinds of adherends, glass and platinum, and 30 kinds of metal elements. From 600,000 possible combinations, we extracted chromium, titanium, cobalt and yttrium as materials showing high adhesion strength data for both glass and platinum. Out of these four types, we narrowed it down to two types, chromium and titanium, excluding cobalt and yttrium, which are expensive, considering the cost aspect. Then conducting just two experiments to verify the strength of the adhesive layer. When factoring in the amount of time spent acquiring necessary information from reference documents and the number of verification experiments required, we were able to reduce the total number of processes by more than 90%.

2. Using MI to search for optimal conditions such as material combination ratios and manufacturing processes

In the past, determining optimal conditions for materials used in development, including ideal combination ratios, volumes and temperatures, involved numerous repeated experiments. However, MI makes it possible to determine such conditions efficiently by picking out candidates for required experimentation in advance based on past experimental data.
In this PoC, we used MI to research four optimal conditions required when designing the adhesive layer, which reduced the number of experiments required by approximately 80%. The results are shown in the table below.

Four optimum conditions in the adhesive layer

Combination Ratio (Chromium : Titanium)	Oxygen Content	Nitrogen Content	Manufacturing Temperature
0.48：0.52	Zero	Zero	246˚C

Based on the results of the above processes, we added an adhesive layer made of chromium-titanium alloy to the glass substrate at 246ºC when forming the platinum film, then verified that peeling did not occur at room temperature or at a high temperature of 800ºC.

3. Reducing CO_2 Emissions

By using MI and CI, the numbers of experimentations are reduced in series of steps from selecting optimal materials to searching for optimal conditions. So compared with conventional method, this process using MI and CI reduced the amount of CO_2 emissions from 1.77 tons to 1.42 tons — a reduction of 0.35 tons*2 ,then contribute to carbon neutrality and achieving at decarbonizes society.

*2 Calculated based on the Guidance on Calculation and Reporting of Avoided Emissions issued by the WBCSD (World Business Council for Sustainable Development). The amount of reduction depends on the evaluation conditions and the evaluation model.

This content is supposed to be presented at the spring meeting of the Japan Institute of Electronics Packaging at Noda Campus of Tokyo University of Science on the 13th of March, 2024.

Hitachi High-Tech is providing solutions that contribute to resolving challenges faced by manufacturing companies, as well as working to create new social and environmental value and contributing toward the realization of a sustainable society.

About CI

https://www.hitachi-hightech.com/global/en/products/ict-solution/randd/ci/

A cloud service provided by Hitachi High-Tech to aid in the discovery of chemical compounds. Supports customers by searching for compounds with a combination of investigative AI and a unique database comprising 43 million English-language patents and other public data.

About MI

https://www.hitachi-hightech.com/global/en/products/ict-solution/randd/mi/

A service and analytics platform provided by Hitachi High-Tech and Hitachi, Ltd. use AI to maximize material properties by deriving optimal combination ratios and manufacturing conditions, contributing to the development efficiency of our customers.

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About Hitachi High-Tech Corporation

Hitachi High-Tech Corporation, headquartered in Tokyo, Japan, is engaged in activities in a broad range of fields, including manufacture and sales of clinical analyzers, biotechnology products, and analytical instruments, semiconductor manufacturing equipment and analysis equipment, and providing high value-added solutions in fields of social & industrial infrastructures and mobility, etc.

The company's consolidated revenues for FY 2022 were approx. JPY 674.2 billion. For further information, visit https://www.hitachi-hightech.com/global/en/

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