A Combinatorial Approach to Opening Unexplored Fields in Metallurgy

Introduction

Today, the requirements for technical surfaces are characterized by a combination of a variety of properties, like hardness, toughness, scratch-proofness, corrosion resistance, wetting, catalytic properties and others. In most cases there are actually no conventional materials available satisfying such complex specifications. Moreover, the latter can not be met by incremental progress in existing materials. The only way to face these specifications is by identifying substantially novel materials. Unfortunately, in view of the tremendous possibilities provided by nature, the "one-at-a-time" approach for finding and testing suitable materials is too slow; hence, new materials with suitable surface properties are rarely found and more rarely optimized. An alternative approach is the combinatorial preparation and testing of surfaces, which includes a screening of compositional and phase gradients of coatings.

Combinatorial Screening and Synthesis of Metallic Materials

Potential Benefits

This method is not in contradiction with existing approaches. The combinatorial synthesis and screening efficiently completes basic knowledge generated by physics, chemistry, metallurgy and materials science and engineering. It allows for fast and efficient screening of materials families identified by these scientific fields as to contain promising solutions to meet technological, environmental and societal specifications.

Challenges

In order to solve all theoretical and technical problems connected to the interdisciplinary field of combinatorial preparation and screening of multifunctional surfaces, expertise in the following topics has to be found and combined: processing, elucidation of surface properties, mechanical properties, phase compositions as well as the modelling and simulation of processes and properties. To achieve this, a group of experts has been established within C-MAC. The group structure and competences allow addressing industrial requirements for technical surfaces based on real life applications.

The C-MAC Organization

C-MAC, the European Integrated Centre for the Development of Metallic Alloys and Compounds has been recently created as a long lasting structure, and as the successor of the European Network of Excellence on Complex Metallic Alloys, NoE CMA. Sixteen universities or national research institutes - covering 20 high level laboratories and one SME - located in ten different European countries, are currently members of C-MAC.

C-MAC's Achievements

The adopted strategy consists in proceeding to the deposition on a Si-wafer by PVD of a composition gradient coating, followed by thorough analysis of phase compositions and surface properties by state of the art instruments. The composition with the highest wetting angle was identified. Homogeneous coatings were prepared with the same composition and showed the same level of properties throughout the sample surface.

Exemplary results of combinatorial preparation of Al-Cu-Fe with a focus on wetting angles:

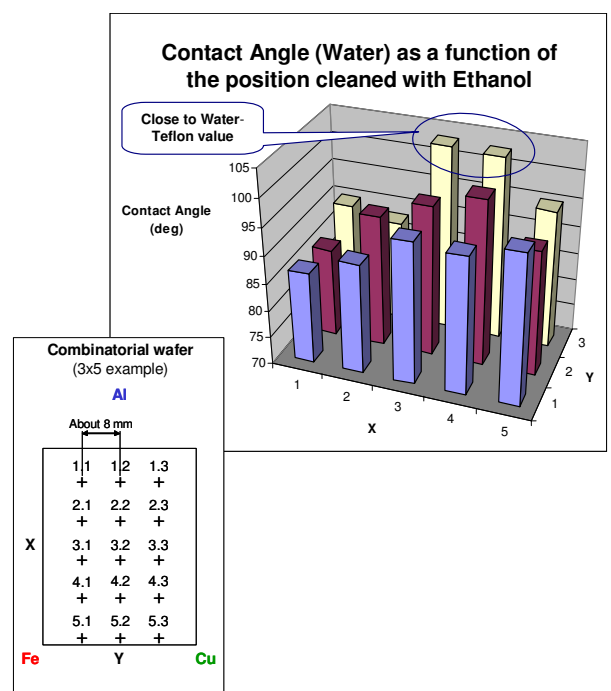**Combinatorial wafer**
(Al Fe Cu gradients)

	1.1	1.2	1.3
Al	60,2	60,2	59,9
Fe	13,2	12,9	13,1
Cu	26,6	26,9	27,0

	2.1	2.2	2.3
Al	52,7	52,5	52,1
Fe	16,7	16,9	14,8
Cu	30,6	30,9	33,0

	3.1	3.2	3.3
Al	47,1	46,8	47,0
Fe	19,3	18,6	16,1
Cu	33,5	34,6	37,9

	4.1	4.2	4.3
Al	40,3	39,5	38,5
Fe	22,7	19,2	17,2
Cu	37,0	41,3	43,3

	5.1	5.2	5.3
Al	36,4	35,8	34,3
Fe	21,2	20,1	16,5
Cu	42,4	44,2	49,2

Combinatorial wafer
(3x5 example)

Al

About 8 mm

```
      1.1  1.2  1.3
       +    +    +
      2.1  2.2  2.3
       +    +    +
 X    3.1  3.2  3.3
       +    +    +
      4.1  4.2  4.3
       +    +    +
      5.1  5.2  5.3
       +    +    +
Fe         Y         Cu
```

Contact Angle (Water) as a function of the position cleaned with Ethanol

Close to Water-Teflon value

Contact Angle (deg)

Combinatorial Screening and Synthesis of Metallic Materials
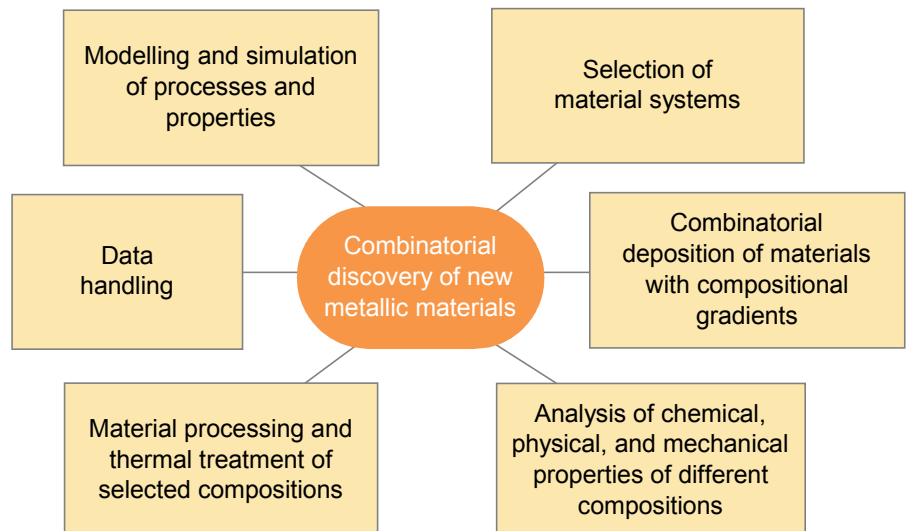
Mission of C-MAC

The main objective of C-MAC is to promote collaborative research in the field of metallic alloys and compounds at a European level. To this end, research is focused on ambitious scientific targets, both on basic and application oriented research.

The Principle of Combinatorial Synthesis and Screening

The approach consists of three subsequent steps:

1. Pre-selection of suitable material systems, according to the output of the ongoing research both on materials for targeted applications and on novel alloy and/or ceramic phases, and according to their field of application and desired combination of properties
2. Deposition of compositional gradients of the material by PVD or CVD methods and the local analysis of their physicochemical and microstructural characteristics and of the targeted properties. Matching of the compositional with the properties gradients over the coating area
3. Selection and homogeneous deposition of suitable target compositions, followed by in-depth analysis of their properties.

C-MAC's Competences

Material Systems
◆ Al-Cu-Fe
◆ Al-Cr-Fe
◆ Binary and ternary metallic alloys
◆ Intermetallics
◆ Nitrides, oxides, carbides of various metals

Processing Techniques
◆ PVD
◆ MOCVD
◆ Inclusion of post deposition thermal treatments

Analytical Methods
◆ Elemental and phase composition: DRX, EDX, Auger, XPS, EPMA
◆ Surface and mechanical properties: (anti-)wetting, hardness, wear, friction, optical properties

Modelling
◆ Modelling in combinatorial and uniform deposition conditions
◆ Thermal and fluid flow profiles
◆ Process probing and modelling
◆ Simulation of operating conditions

Other Competences
◆ Data management and mining

Combinatorial Screening and Synthesis of Metallic Materials

European C-MAC

Industry Support Group (ISG)

C-MAC offers ISG members a novel way to utilize the latest scientific findings and technological results in the field of CMA. Depending on the membership class, an ISG member can participate at the Science Board Meetings to discuss strategic issues such as long-term research activities, and will get information about ongoing research. Additionally, participation in common PhD programmes or joint research projects, organized individually on a case-by-case basis, is offered.

This looks like a promising approach, but ...

... how can you get hold of the latest research results?

... how can you influence the direction of research?

... where is the specialist who answers your questions?

... who builds the bridge between academic research and your development?

**Many questions - one answer:
join the Industry Support Group!**

Contact us for more information

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