IRES
Innovation in Research & Engineering Solutions

Advances and challenges of Safe-and-Sustainable-by-Design (SSbD) The case of high-entropy alloy (HEA) coatings

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Presentation Outline

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  - The SSbD framework
- **Objectives**
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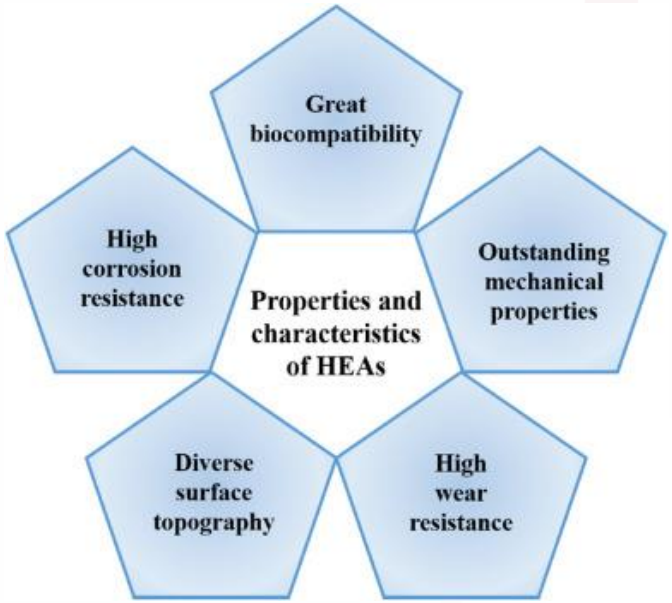
Introduction

High Entropy Alloys (HEAs) and coatings

- **What are high-entropy alloys?**

High entropy alloys (HEAs) are a novel class of materials that are composed of **at least five principal metallic elements**.



The global high-entropy alloy **market size** was USD 54.7 million in 2022 and the market is projected to reach USD 202.97 million by 2028, showcasing a compound annual growth rate **(CAGR) of 24.42%** during the forecast period.

- **Why are they important?**

HEAs show **unique properties** at surface modification and **coating**.

- **How do we fabricate HEA coatings?**

Three main methods: Vapor deposition, Thermal spraying and Laser deposition. **Physical vapor deposition** coating, also known as thin-film coating, uses a vacuum chamber to vaporise a solid and deposit it onto a target substrate, atom by atom.

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Sources: https://doi.org/10.1016/j.smmf.2022.100009, https://www.businessresearchinsights.com/market-reports/high-entropy-alloy-market-110243, https://doi.org/10.1016/j.jestch.2022.101211 https://korvustech.com/what-is-pvd-coating/, https://korvustech.com/sputtering/, https://korvustech.com/magnetron-sputtering/

Introduction
The SSbD framework

Safe-and-Sustainable-by-Design (SSbD) framework is designed to evaluate new and existing chemicals / materials and **minimize negative impacts** on **human health** and the **environment.**

To **guide the innovation process** towards **safe** and **sustainable** new materials

- ✓ Steer the **innovation process** towards the green and **sustainable** industrial transition.
- ✓ **Substitute** or minimize the production and use of **substances of concern**
- ✓ Minimize the **impact on health**, **climate** and the **environment** .

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Source: https://research-and-innovation.ec.europa.eu/events/upcoming-events/safe-and-sustainable-design-boot-camp-2023-10-25_en

Objectives
of the methodology

Purpose

Examination of **safety** and **sustainability** level of high-entropy materials.

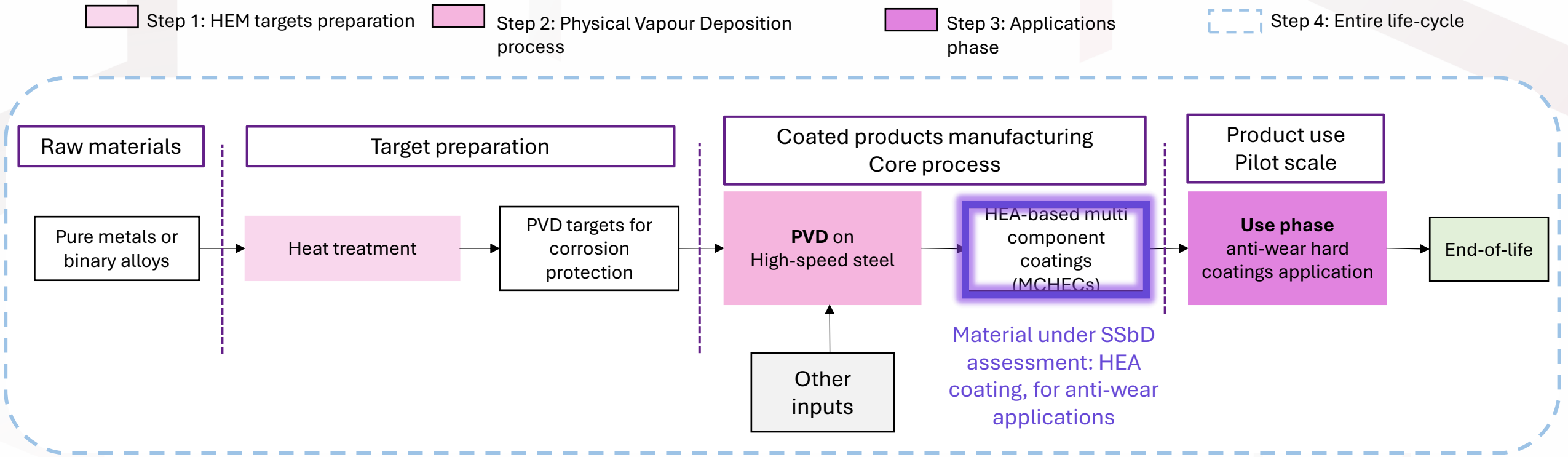
How?

Through the newly developed five-step **Safe-and-Sustainable-by-Design** framework.

Why?

- To support the **design** and **development** of safe and sustainable High-Entropy-Materials (HEMs).
- To provide a comprehensive **evaluation of the applicability of the SSbD** methodology to the production of novel HEMs and their use as coating materials.
- To identify any **gaps** and **limitations** of the framework
- To provide **additional value** to the concept of safety and sustainability to the materials industry.

Case study
Production process of high entropy coatings



M2DESCO **simplified process** for SSbD example application

Case study
The 5-step framework

Design principles

Increasing Technology Readiness Level (TRL)

Synthesis → Scaled-up Manufacturing → Pilot scale manufacturing

Safe-and-Sustainable-by-Design Chemical / material

Safety and sustainability assessment

1. Hazard assessment of chemical / material
2. Human health & safety aspects in production and processing
3. Human health and environmental aspect in use phase
4. Environmental sustainability assessment
5. Social and economic sustainability assessment

Step 5 is under development and will not be assessed in this study

Case study

Step 1: Hazard assessment of the chemical/material (intrinsic properties)

Step 1 aims to identify appropriate **criteria** based on **intrinsic properties** applied during the **(re)design** of chemicals and materials

STANFORD ADVANCED MATERIALS

Material (M=Alternative metals)	SSbD score Step 1
Benchmark (AlTiN)	
FeCrNiMnAl**M**	

Material	SSbD score Step 1
AlTiN	?
Fe	
Cr	
Ni	
Mn	

Observations

- Lack of data, for novel materials especially
- Pure elements assessment accuracy is debatable – alloy matrix shall be considered (REACH)
- Uncertainty of available information (e.g. Cr, Fe, FeCr). Specific information from suppliers is essential.
- Confidentiality issues for advanced materials

Hazard classification & labelling **Fe**

Danger! According to the classification provided by companies to ECHA in **REACH registrations** this substance is self-heating and may catch fire and is a flammable solid.

Breakdown of all 5857 C&L notifications submitted to ECHA

Not Classified	
Self-heat. 1	H251
Flam. Sol. 1	H228
Eye Irrit. 2	H319
STOT SE 3	H335
STOT RE 2	H373

Hazard classification & labelling **Cr**

According to the notifications provided by companies to ECHA in REACH registrations no hazards have been classified.

No harmonised classification

Additionally, the classification provided by companies to ECHA in **CLP notifications** identifies that this substance is very toxic to aquatic life, is very toxic to aquatic life with long lasting effects, causes serious eye irritation, may cause an allergic skin reaction and may cause allergy or asthma symptoms or breathing difficulties if inhaled.

ECHA EUROPEAN CHEMICALS AGENCY

e.g. evidence on **Cr** and **Fe** vs evidence on **FeCr**

WARNING

Ferrochromium (FeCr)

H317: contact with skin may cause skin allergic reaction.
H373: Can affect respiratory organs after multiple or continuous exposure;
H413: Can cause continuous hazardous effect on aquatic life [17].

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Sources: https://echa.europa.eu/substance-information/-/substanceinfo/100.028.324, https://rfainternational.com/wp-content/uploads/2016/11/MSDS_FeCr_eng_2016-2021.pdf

Case study

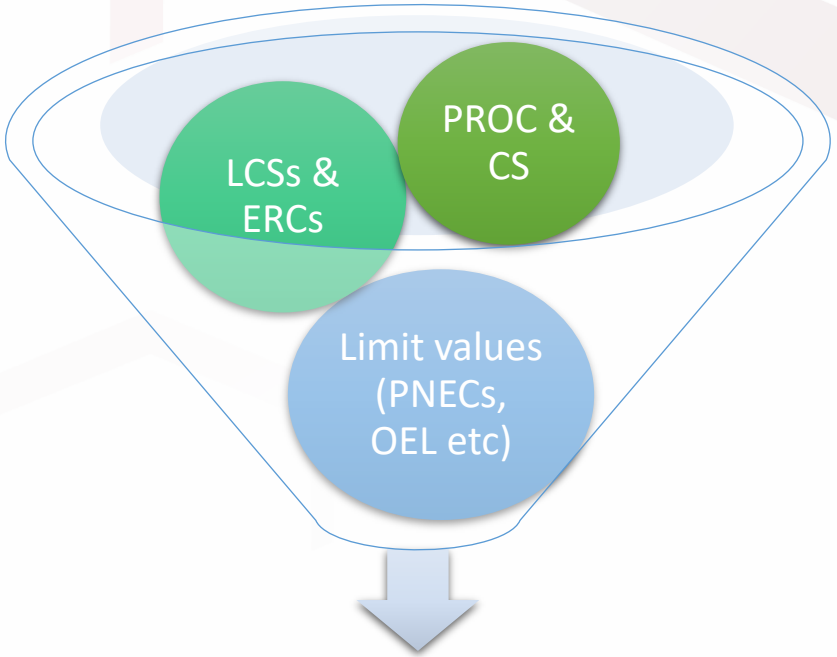
Step 2 **&** 3: Human health and safety aspects in the production and processing phase **&** human health and environmental aspects in final application phase

ECHA recommends **Chesar**
(built-in ECETOC TRA and EUSES)

Recommended tools by JRC

Table R.14- 2: Applicability matrix (inhalation models)

Applicability	ECETOC TRA	MEASE	EMKG-EXPO-TOOL	STOFFENMANAGER	ART
PROC codes (as input)	Yes	Yes	No	No	No
Covered physical state	Solid /liquid=volatile	Solid /liquid	Solid /liquid	Solid /liquid	Solid /liquid
Beyond scope	• Fibres • aerosol mist • emissions from • hot processes (e.g. fumes) • gases • caution needs to be exercised when applying to CMRs and very high hazard substances • solids in liquids	• organic substances • some restrictions concerning special combinations of PROC/physical properties	• Dusts by abrasive techniques, • fumes (soldering, welding, acid fumes) • gases • open spray • pesticides • wood dusts • CMR substances	• Fibres • gases or hot working • techniques (welding, soldering, • acid fumes)	• Dust resulting from emissions during hot metallurgical processes • fibres • fumes • gases • solutions of solids in liquids
Basis of use description	process based	process based	task based (control guidance sheets)	task based	task based



Risk Characterisation Ratios

$$RCR = \frac{\text{Predicted concentration}}{\text{Limit value}}$$

PECs: Predicted Environmental Concentrations
PNEC: Predicted No-Effect Environmental Concentrations
OEL: Occupational Exposure Limit
RCR: Risk Characterisation Ratio

LCS: Life Cycle Stages
ERC: Environmental Release Category
PROC: Procedure
CS: Contributing Scenario

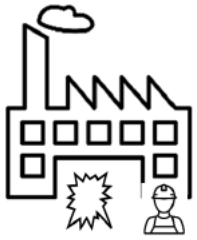
Source: ChemSafetyPro_Toxicology & Health Risk Assessment

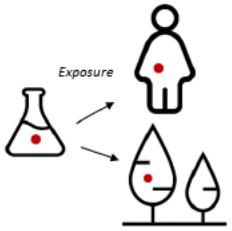
Case study

Step 2 & 3: Human health and safety aspects in the production and processing phase & human health and environmental aspects in final application phase

Observations

- Exposure estimation tools have **limitations** to their domain of applicability
- Complexity of tools use – need for training and / or support
- Lack of **data** – extensive input required by tools to generate results
- Low availability of use maps
- Manual input of information is a time-consuming process – need for automated system
- **Uncertainty** of assessment regarding the default **procedure categories** and contributing scenarios – need for training and multi-disciplinary synergies
- Default exposure and release factors lead to conservative results.



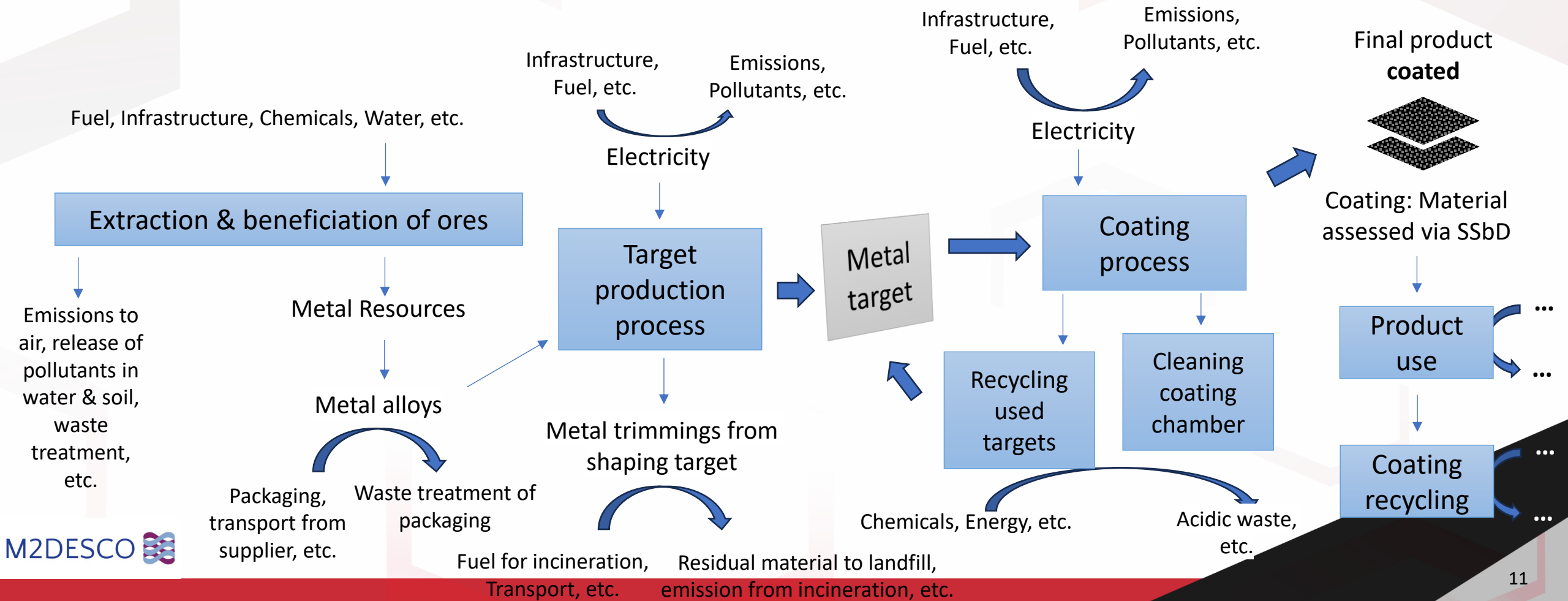


Source: https://research-and-innovation.ec.europa.eu/events/upcoming-events/safe-and-sustainable-design-boot-camp-2023-10-25_en

Case study

Step 4: Environmental sustainability assessment along lifecycle

Unlike Steps 1-3, which focus only on the material being investigated, Step 4 **considers all the inputs and outputs** within the system boundaries, along the entire lifecycle of the material.



Case study

Step 4: Environmental sustainability assessment along lifecycle

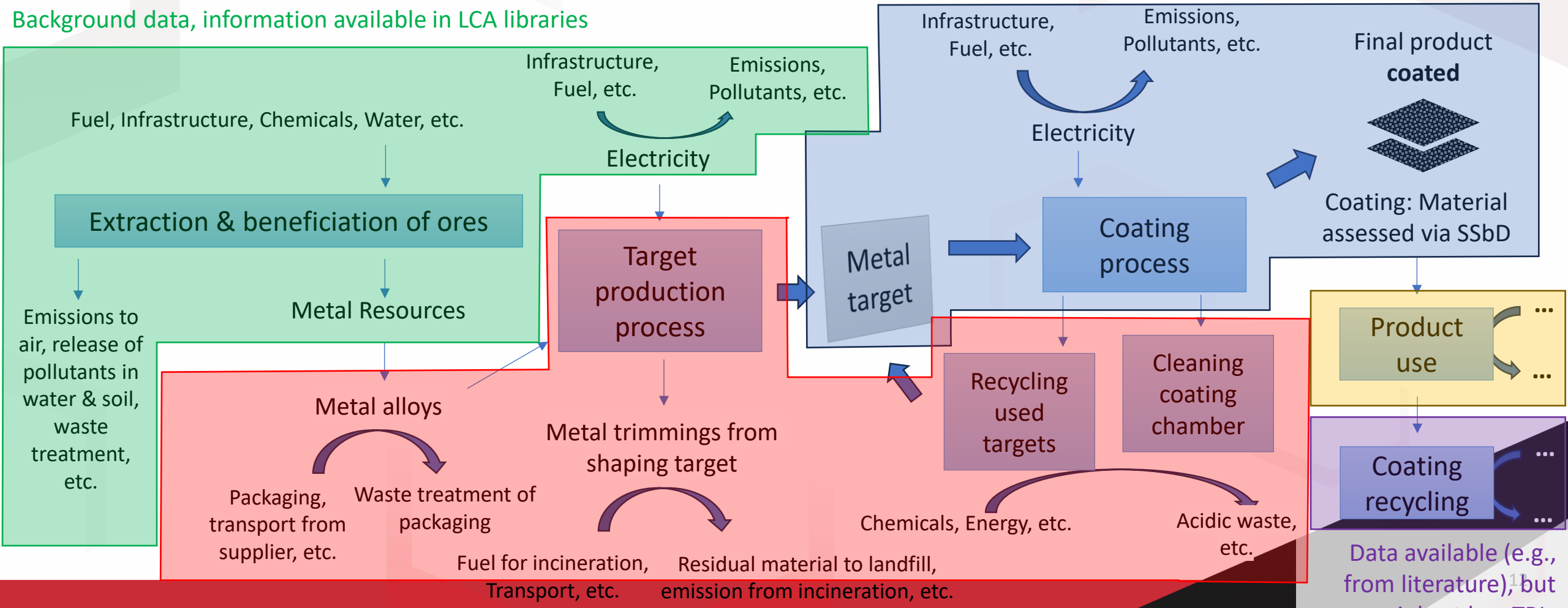
Commercial data, confidential.

Data availability depends on the product

Background data, information available in LCA libraries

Main limitation for Step 4: **Lack of data**

Foreground data: accurate information from project partners



Data available (e.g., from literature), but mainly at low TRL

Take-home message

… concerning the case of HEA/HEC

Available tools have limitations on their scope and applicability.
Need for one integrated tool to address the whole framework.

Complexity of framework and online tools that provide estimations. Need for in-depth training.

SSbD framework through **the 5-steps puts together the most essential aspects** towards a safer and more sustainable material

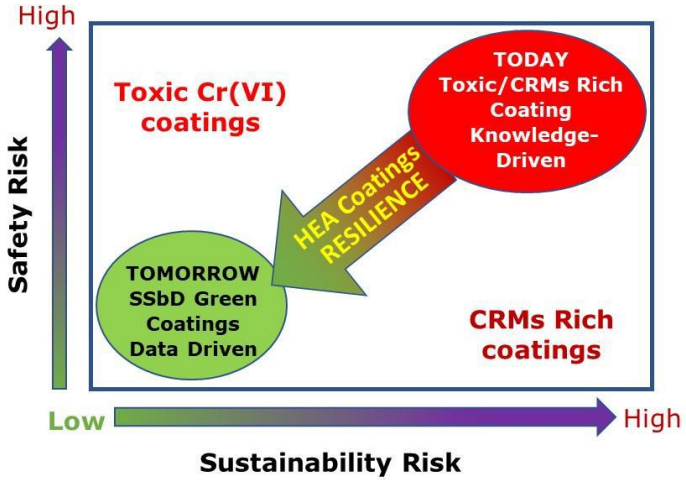
Interdisciplinary framework, difficult to apply by one person.
Need for multi field experts' cooperation.

Lack of available data in literature.
Partners should provide specific information per case of application.

Computational Multi-Models Enabled Design of Safe & Sustainable Multi-component HEA

M2DESCO partners

The **aim of the project** is to develope tools with enhanced properties by introducing green, safe and sustainable **multi-component high entropy coatings.**



Integrating all the above into **AI** and **machine learning** tools, a data driven, decision-making tool will be created, that will lead to **safe-and-sustainable-by-design** solutions, following the framework's guidelines.

IRES short description & team

IRES is an R&D consulting company, established in 2015, that provides specialized services in the fields of:

- Sustainability & Circularity
- Risk &(nano)Safety
- Data Science & Materials Science Digitization

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Thanks for your attention

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