SAFE AND SUSTAINABLE BY DESIGN GRAPHENE/MXENES HYBRIDS

Safe and sustainable by design (SSbD) production of Niobium MAX Phases and MXenes

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INTRODUCTION & OBJECTIVES

- MXenes are layered transition metal carbides, carbonitrides, and nitrides produced from layered ternary materials known as $M_{n+1}AX_n$ or MAX phases by selective etching the A-layers.
- SAFARI project main objective is the safe and sustainable by design (SSbD) production and utilization of MXenes, covering the whole supply chain, starting from the precursors' preparation (MAX phases), MXenes production and functionalization and going to end applications (Figure 1).
- A sustainable production route for the preparation of high-quality and highpurity MAX phases based on the combination of Spark Plasma Sintering (SPS) and High Energy Ball Milling (HEBM) has been adopted to produce Niobium MAX phases (Nb_4AlC_3). Next, Niobium MXenes (Nb_4C_3) were obtained via High Frequency Acoustic Emission (HFAE), a fast and environmentally friendly process, assisted by Chemical Digestion (CD) as source of heat for the MAX phases etching.

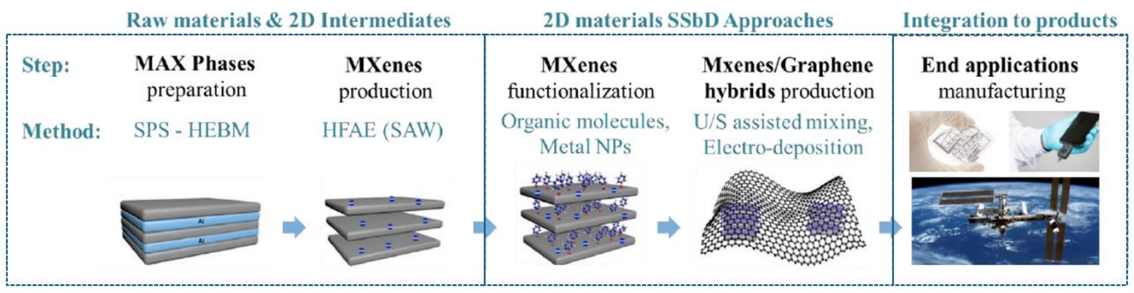

Figure 1.– SAFARI´s SSbD MXenes supply chain.

- The objective of this study is to determine the environmental and economic impacts of MAX phases and MXenes production via LCA and LCC assessments in order to identify hotspots and improvement opportunities, thereby supporting the innovation process.

METHODOLOGY

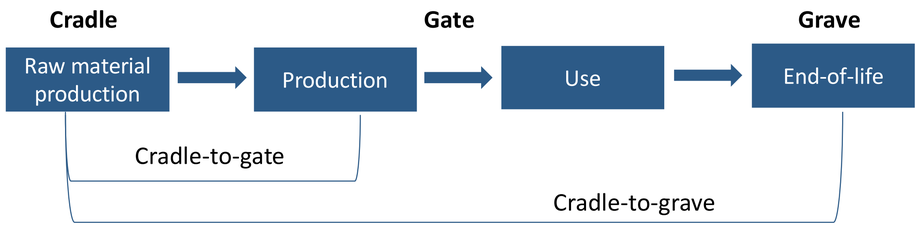

Figure 2.– Scope selected for LCA : Cradle-to-Gate.

LCI data consisted of primary data obtained from the production process data provided by Łukasiewicz Research Network – Poznań Institute of Technology (PIT) partners. This data included inputs, outputs, wastes, energy requirements and equipment involved in the production processes and their costs.

To determine the environmental impacts, a Life Cycle Assessment (LCA) was carried out following ISO 14040/14044 and PEF methodology. The software SimaPro v10.1 with the database Ecoinvent 3.10 and the Environmental Footprint v3.1 method were used.

To determine the economic impacts, a Life Cycle Costing (LCC) was carried out following SETAC/UNE-EN 60300 guidelines. Economic impacts were calculated using an excel spreadsheet with the exception of the environmental externalities, calculated using SimaPro 10.1 software with the European Environmental Prices method.

The functional unit was 1 g of manufactured material (MAX phase or MXene), and the scope was Cradle-to-Gate (Figure 2).

The goal is to identify the primary environmental and economic impacts associated with the MAX Phases and MXenes materials production.

RESULTS & DISCUSSION

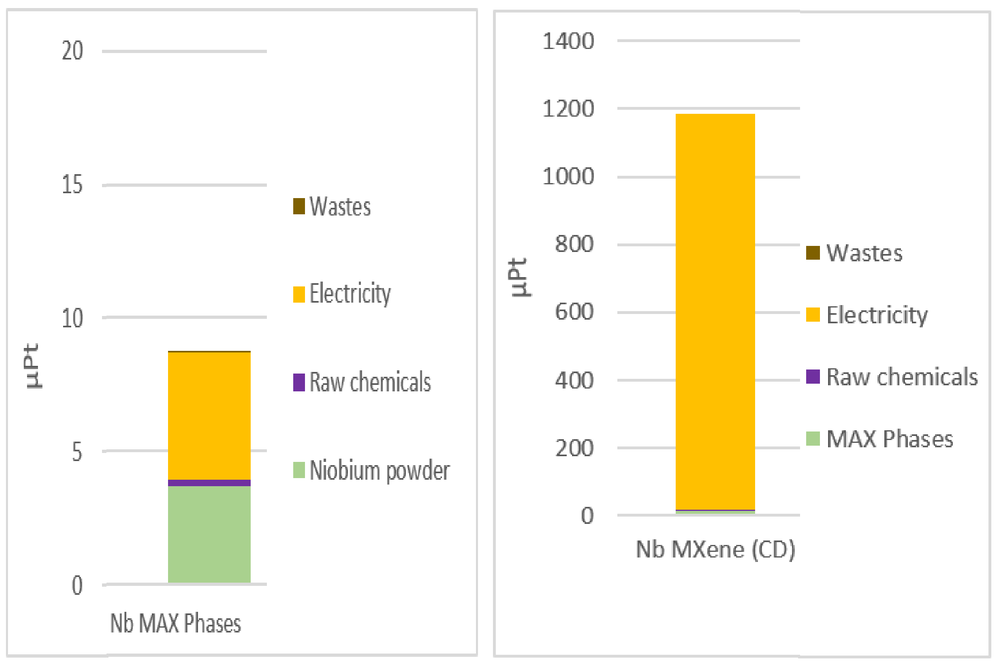

Figure 3.– MAX Phases (left) and MXenes (right) Environmental impact.

Economic impact

- Regarding MAX phases production: the cost of niobium powder becomes the dominant cost driver, accounting for 79% of the total, followed by direct manufacturing costs (17%) which mainly arise from the labour-intensive nature of the process.
- Nb_4C_3 MXenes production: the raw materials is the main cost driver, especially owing to the ammonium bifluoride (NH_4HF_2) which is responsible for the 50% of the total costs, followed by Labour costs (33% of the total).

Environmental impact

- Regarding MAX phases production: the energy consumption represents 54% of the impacts with the high energy ball milling and the spark plasma sintering as the main contributors. The Niobium powder production represents other 42% of the total. The most concerning impact categories are Climate change followed by Resource use, fossils.
- Nb_4C_3 MXenes production: the electricity is the main hotspot, providing 98% of the total environmental burdens. The most concerning impact categories are Resource use, fossils followed by Climate change.

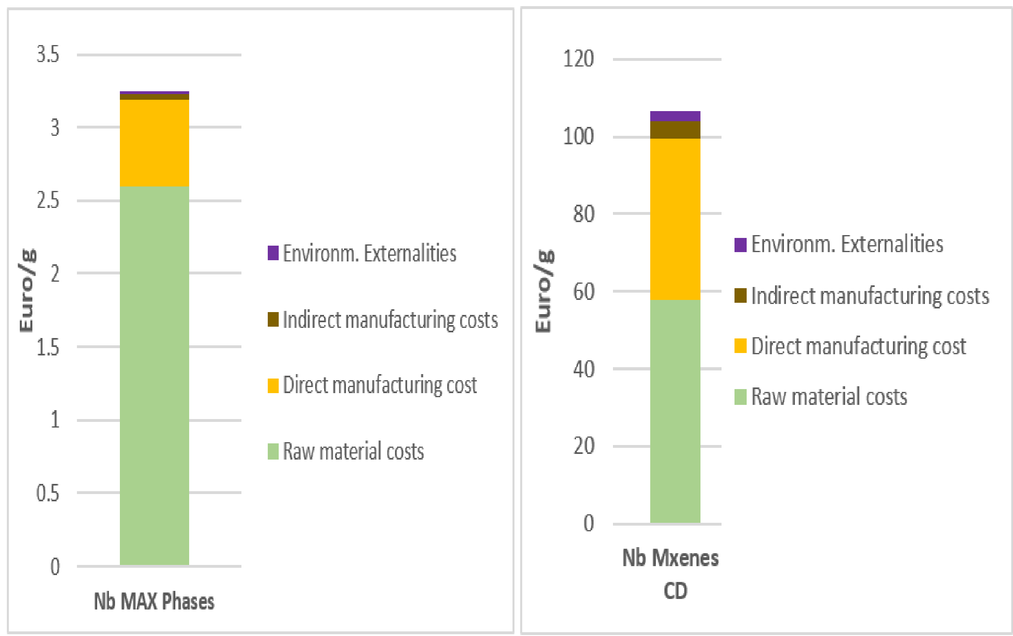

Figure 4.– MAX Phases (left) and MXenes (right) Economic impact.

CONCLUSIONS

As energy consumption in the production processes is the primary cause of environmental impact, further improvements should be focused on reducing the upstream burdens related to the electricity production by selecting more sustainable sources. However, it is recommended to continue working on obtaining higher energy efficiency. Labour costs were highlighted as an economic hotspot, which is expected to be reduced with the upscaling of the process. Regarding raw materials cost, for NH_4HF_2 it is recommended to reduce its equivalents as much as possible or maybe find alternative fluoride sources for the etching process.

ACKNOWLEDGEMENTS

GRAPHENE FLAGSHIP

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SAFARI PROJECT

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