SAFE AND SUSTAINABLE BY DESIGN OF GRAPHENE AND MXENES HYBRIDS

Safe and sustainable by design (SSbD) MAX Phases and MXenes: environmental impacts comparison through Life Cycle Assessment (LCA)

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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, 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 in order to produce 2 MAX phases: Ti_3AlC_2 and Cr_2AlC. Next, Ti_3C_2 and Cr_2C MXenes can be obtained from their corresponding MAX phases via High Frequency Acoustic Emission (HFAE), a fast and environmentally friendly process. Chemical digestion (CD) and microwave (MW) as sustainable source of heat were used for the MAX phases etching.

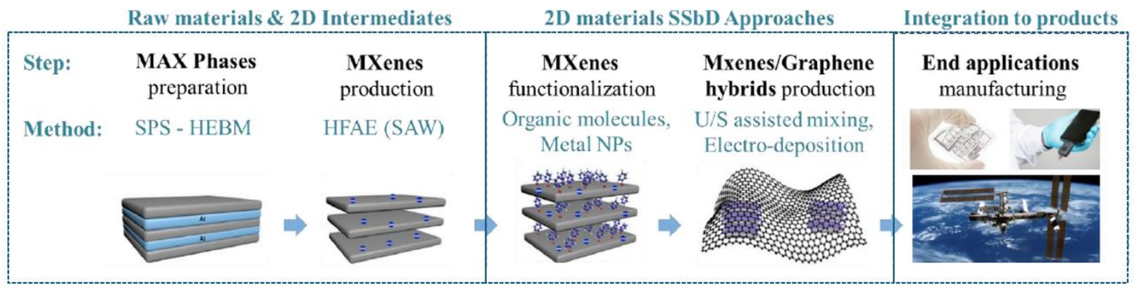

Figure 1.– SAFARI´s SSbD MXenes supply chain.

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

METHODOLOGY

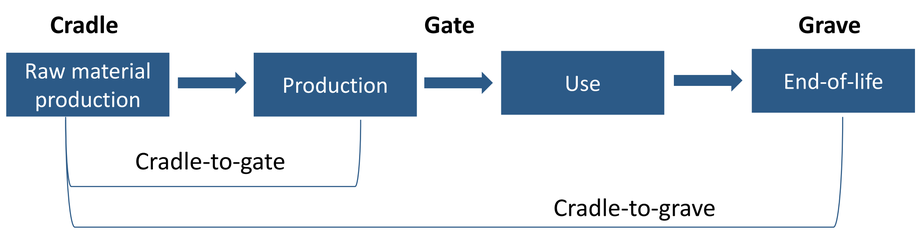

Figure 2.– Scope selected for LCA : Cradle-to-Gate.

To determine the environmental impacts, an LCA was carried out following ILCD handbook and ISO14040 methodology. The software SimaPro v9.6 with the database Ecoinvent 3.10 and the Environmental Footprint 3.0 method were used. The functional unit was 1 kg of manufactured material (MAX phase or MXene), and the LCA scope was Cradle-to-Gate (Figure 2).

The goal is to identify the primary environmental impacts associated with the MAX Phases and MXenes materials production. Regarding MAX phases, the production process of Ti_3AlC_2 and Cr_2AlC were assessed and compared. Regarding MXenes, 2 different MAX phases etching process (CD and MW), used to obtain MXenes, were compared.

The data for the LCI 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 and energy requirements of the production processes of MAX phases and MXenes.

RESULTS & DISCUSSION

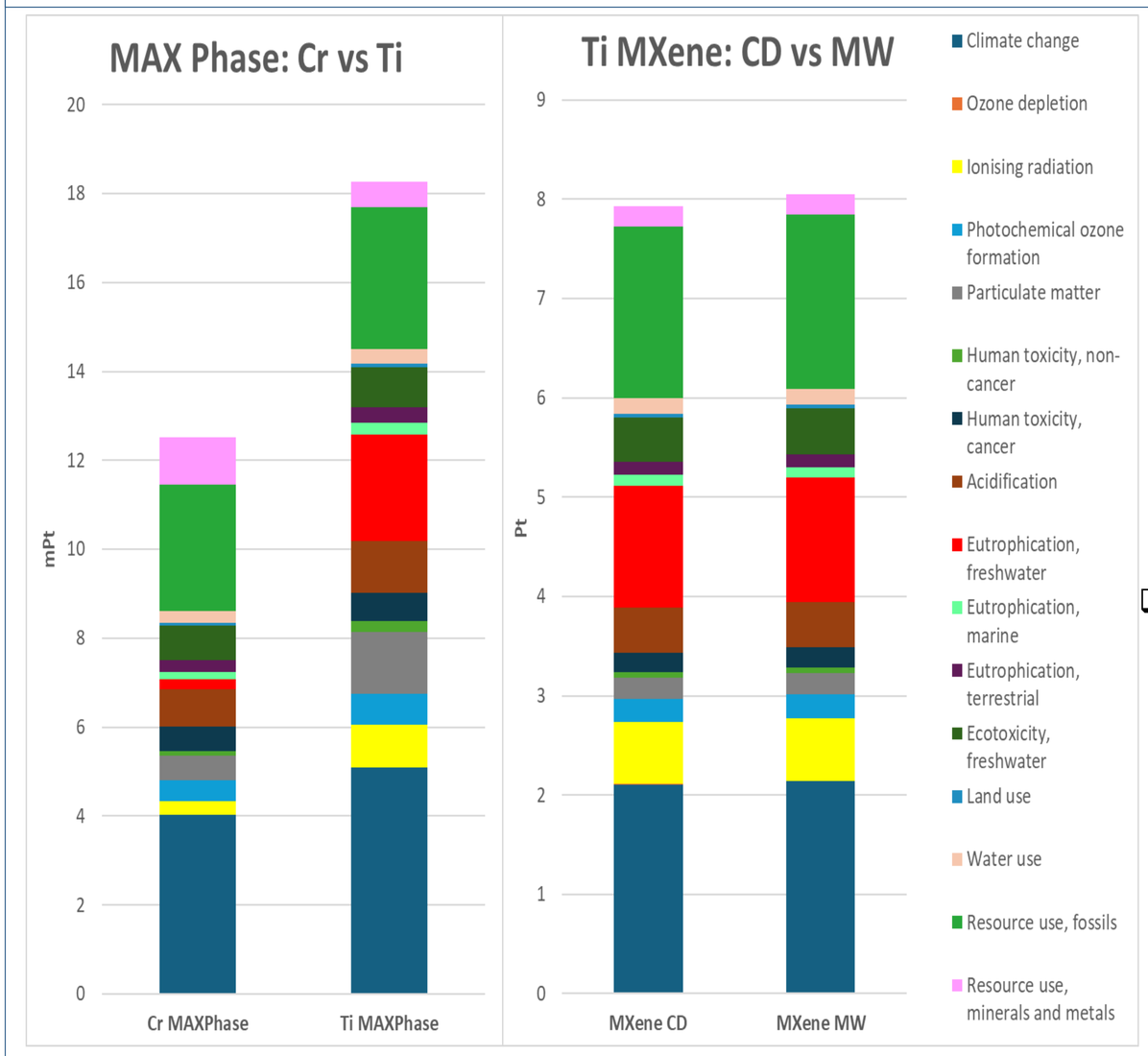

Figure 3.– MAX Phases Environmental impact (left) and MXenes Environmental impact (right).

- Regarding MAX phases production: Ti_3AlC_2 has a greater environmental impact than Cr_2AlC (higher by 1.5 times). In both MAX Phases, the category with the highest environmental impact is Climate change followed by Resource use, fossils (1.3 and 1.1 times higher in Ti_3AlC_2, respectively). In the case of Ti_3AlC_2 , the next highest impact categories are Eutrophication, freshwater and Particulate matter, while for Cr_2AlC are Resource use, minerals and metals and Acidification.
- Ti_3C_2 MXenes were produced by Ti_3AlC_2 etching via CD and MW, being the environmental impact of these MXenes very similar. In both cases, the order of the categories with the highest environmental impact is: Climate change followed by Resource use, fossils, Eutrophication, freshwater and Ionising radiation. Being practically the same order as in the case of the MAX Phase.
- Electricity is the process that contributes most to the environmental impact in the production of both MAX phases and MXenes.

Figure 4.– MAX Phases (left) and MXenes (right) Process contribution.

CONCLUSIONS

The study has shown that the choice of the metal to be used in the MAX Phase is of great importance in relation to the environmental impacts that the production process of these new materials can cause. The impact categories with the highest environmental impact are Climate change followed by Resource use, fossils in both MAX Phases and MXenes production, being electricity the process that contributes most to the environmental impact.

ACKNOWLEDGEMENTS

GRAPHENE FLAGSHIP

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