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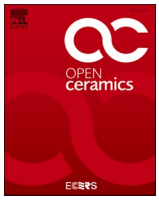

Cost analysis of MXene for low-cost production, and pinpointing of its economic footprint

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ABSTRACT

MXene, a two-dimensional (2D) carbide, carbonitride, and nitride, was discovered in 2011. A certain number of elements in the periodic table have contributed to the synthesis of MXene from the beginning to the present. Most researchers, however, are focused on a particular type of MXene, $Ti_3C_2T_x$, although the scientific community seldom considers the synthesis cost of this outstanding and potentially helpful substance. Herein, we explore the cost of MXene by going through each stage of the production process. Instead, the actual cost may vary by a small margin due to differences in the materials and procedures. However, this study provides a clear understanding of the cost, which is governed by the steps directly involved in the synthesis and characterization of MXene. The cost associated with various essential characterization tools like scanning electron microscope (SEM), transmission electron microscope (TEM), ultraviolet–visible spectroscopy (UV–Vis), and x-ray diffraction (XRD) is necessary to ensure the successful synthesis of MXene. All local expenses are converted into USD, except for the instrumental life cycle analysis and infrastructure cost values. The cost of each gram of MXene is predicted to be $20.33. The predicted cost is close to the market price of MXene, proving the accuracy of the cost calculation presented in this research. This work will assist the scientific community in planning and optimizing MXene's synthesis procedures so that the production cost can be potentially reduced if this material is produced on a larger scale.

1. Introduction

MXene is a two-dimensional (2D) material belonging to the category of carbides, carbonitrides, and nitrides. MXene is produced by selectively etching an A layer from the MAX phase, which primarily consists of ternary carbides or nitrides. The general formula for MXene is $M_{n+1}AX_n$, where M represents an early transition metal, A represents group III or IV elements, X is C or N, and n = 1 to 4 [1]. The selective etching process removes the bonded $M_{n+1}X_n$ layer without affecting the M-X bond, and sonication has been found effective for this purpose. Moving on to the procedures, the first step involves selecting the precursors for MXene synthesis, known as MAX phase materials, typically comprising ternary carbides or nitrides of transition metals with the formula $M_{n+1}AX_n$. M stands for an early transition metal, A for an element from group IIIA or IVA in the periodic table, X for either carbon or nitrogen, and n for 1, to 4. Etching the A layer from the MAX phase is the primary route to synthesize MXene, $M_{n+1}X_nT_n$, which the MXene formula is presented in Fig. 1. The M-A bonds and the M-X bonds in the MAX phase react differently toward an etching reagent during an etching treatment, leading to selective etching of the A layers. The transition metals such as Ti [2], V [3], Cr [4], Y [5], Zr [6], Nb [7], Mo [8], Hf [9], Ta [10], and W [11] are often used for MXene synthesis. Other transition metals, such as Sc [12] and Mn [13] only been discovered theoretically. The M-elements eventually become terminated with surface termination groups (T_n) such as O, and Cl, which are commonly observed [14].

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The precursor preparation for the MAX phase is important [15]. The quality of MXene entirely depends on the quality of the as-synthesized MAX phase. The proportion of each selected precursor (M, A, and X elements) must be optimal. Most researchers choose a ratio based on a careful literature review assessment. The MXene ($Ti_3C_2T_x$) is formed by combining Al and Ti in a specific molar ratio with different carbon precursors. Fig. 2 depicts the sequential steps required to synthesize MXene, starting from the precursors. By inspecting Fig. 2 thoroughly, the synthesis of MXene entails the following procedures: precursors, ball milling, tube furnace, grinding, etching, washing, and drying. Although all the steps are equally essential to ensure successful synthesis, tube furnaces, and etching is particularly crucial. The variables and guidelines for synthesizing MXene are also provided in Fig. 2. The ball mill is used to achieve a homogeneous mixture of the precursor materials, and it is occasionally necessary to alter the shape or decrease the size of the precursors. This powdered blend is then heated in a tube furnace. Finally, the tube furnace is introduced to produce the MAX phase materials. Once the MAX phase material has been removed from the tube furnace, it must be ground into powder using a mortar and pestle or drilling bits before it can be used in the etching process.

The etching process involves the selection of the method and etching chemicals such as LiF [16], HCl [17], HF [18], NH_4HF_2 [19] etc. Since the A atomic layer is removed selectively from the MAX phase, the $M_{n+1}X_n$ layers can be manipulated and tuned to remain unharmed throughout this process. The A atom is oxidized during the etching processing; its nominal oxidation state in the MAX phase is relatively low [15]. After the procedure is finished, the components, which we may now refer to as MXene, must be washed. The purpose of washing these materials is to dilute the etching acid and neutralize the reaction. The mixture of components (unetched and etched MAX phases, excessive salt, and impurities) can be separated via centrifugation since the components have different densities. Distilled water (DI water) and a centrifuge machine are employed and eventually followed by a drying process. To avoid further oxidation of MXene, the sample must be dried in a vacuum oven. One drawback of MXene is that it oxidizes fast in the presence of water and air, depleting the product's potential [15]. Storing the synthesized MXene entails the following procedures: The materials will need to be stored in a vacuum to avoid oxidation. In such instances, a desiccator is utilized to keep the components protected from oxidation while they are stored. While some research suggests that storing MXene in a liquid or frozen state is preferable, the use of a desiccator is the most practical option.

The next step is validating the MXene formation using an electron microscope and x-ray diffraction (XRD) equipment. The morphology of the MXene can be observed by using a scanning electron microscope (SEM). The multi-layered morphology can be further confirmed and revealed by a transmission electron microscope (TEM). X-ray diffraction (XRD) can be employed to validate the crystallographic structure and composition of the MXene. In addition, it is also necessary to examine the samples for UV–Vis [15] and energy dispersive x-ray (EDX) spectra to confirm the nature of MXenes. MXene and MXene-based composites have shown immense potential, particularly in energy storage applications [20]. They have proven especially impactful in catalysis and electronic components [21], due to their strong metallic electrical conductivity, high solubility in water, and distinctive redox properties. MXene also shown great potential in water purification [22–24], due to their good hydrophilicity, surface area, and photothermal conversion efficiency.

Extensive research has been conducted, primarily focusing on $Ti_3C_2T_x$ [25]. The scientific community has extensively examined synthesis procedures, parameters, etching processes, and safety protocols for MXene production from its MAX phase precursors [26–28]. While previous research has predominantly focused on the synthesis and characterization of MXenes, there is a significant research gap regarding the economic aspects and cost considerations of large-scale production. This gap inhibits the commercialization and broader utilization of MXene-based technologies. Understanding the cost factors involved and developing cost-effective synthesis methods are imperative for overcoming these challenges and enabling large-scale utilization of MXenes. Market research [29–31] indicates that MXene powder costs $10.19 per gram [32], significantly lower than graphene at $945 per gram [33], and carbon nanotubes at $201.9 per gram [34], as of 2022. Despite MXene's cost advantage, a comprehensive cost analysis for MXene synthesis is still needed. In this study, we estimate the cost of synthesizing $Ti_3C_2T_x$ MXene, considering all synthesis steps, materials, characterization tests, and labour costs, making this study a valuable guide for researchers to plan and conduct cost-effective scientific investigations and optimize large-scale production for commercial and specific applications.

This research paper aims to address this research gap by discussing a method for calculating the cost of MXene production using the modified acid method, a widely employed approach for synthesizing MXenes from MAX phase precursors. The modified acid method involves the etching of MAX phases using a mixture of lithium fluoride (LiF) and hydrochloric acid (HCl), followed by delamination and washing steps to obtain MXene products [35]. The primary objective of this study is to provide a comprehensive analysis of the process cost associated with MXene production using the modified acid method. The most common method for converting MAX phases into MXenes involves the use of hydrofluoric acid (HF). HF selectively reacts with the A-group element layers (typically aluminium or silicon) in the MAX structure, leaving behind the MXene nanosheets. This approach is widely used due to its simplicity and efficiency, resulting in high-quality MXenes. Alternative etching agents, such as chloride-based solutions (e.g., LiF/HCl), have been explored to mitigate the safety concerns associated with HF. These methods can provide similar results in terms of MXene synthesis and scalability, making them appealing from an environmental and safety perspective. The analysis includes cost components such as raw materials, reagents, energy consumption, equipment, and labour costs. By quantifying these factors, we aim to elucidate the economic feasibility and challenges associated with large-scale MXene production.

Additionally, this study explores strategies for minimizing the cost of MXene synthesis using the modified acid method. Optimization of etching parameters, such as LiF and HCl concentrations, reaction time, and temperature, will be investigated to maximize MXene yield while minimizing reagent consumption. The potential for reagent recycling and recovery will also be explored to reduce overall production costs. Experimental results from a pilot-scale MXene synthesis using the modified acid method will be presented to support the analysis. The

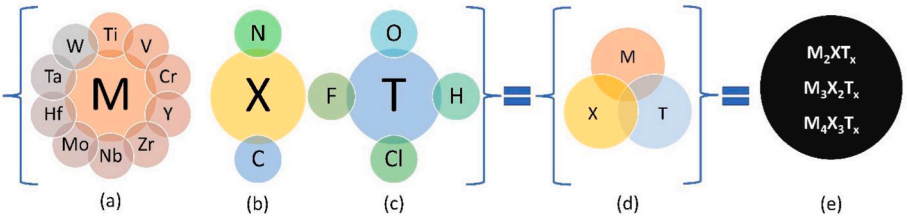

Fig. 1. The formulation configuration of MXene; (a) Transitions metal in MXene; (b) carbon or nitrogen; (c) surface terminations; (d) reaction process; (e) synthesized MXene.

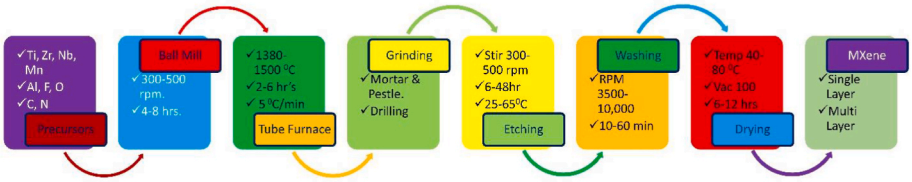

Fig. 2. Flow diagram of MXene synthesis with essential variables.

costs associated with raw materials, reagents, energy consumption, equipment, and labour will be carefully evaluated and compared with existing literature on other MXene synthesis methods to determine the cost advantages and limitations of the modified acid method. The findings of this study will provide valuable insights into the cost-effective production of MXenes and guide researchers and industrial stakeholders in making informed decisions. By identifying cost reduction opportunities and proposing strategies for process optimization, this work aims to contribute to the development of scalable and economically viable MXene synthesis methods. Ultimately, these efforts will accelerate the commercialization of MXene-based technologies, enabling their broader utilization in diverse fields.

2. General methodology

In the realm of material science and industrial applications, a comprehensive cost analysis is imperative for gaining insights into the economic feasibility of a given material. Our methodology seeks to demystify this process by employing a straightforward approach that meticulously accounts for various cost components. Beginning with the basics, we meticulously identify and catalogue all raw materials involved, ranging from precursors to etching agents. This exhaustive list ensures that every contributing factor is taken into consideration. Simultaneously, we delve into the realm of utilities, encompassing electricity and gas consumption. These components, often overlooked, are pivotal contributors to the overall cost structure and warrant thorough examination. The amalgamation of these raw material and utility expenses allows us to calculate the baseline cost of the materials under scrutiny. This holistic approach provides a comprehensive understanding of the financial implications associated with the production process, offering a solid foundation for strategic decision-making. Beyond the tangible components, we extend our analysis to include labour costs. Recognizing the pivotal role of human resources in the production cycle, our methodology accounts for the personnel involved in various stages of the process. This comprehensive consideration ensures that the true cost of material production is transparently reflected in our calculations. It is crucial to note that, in our methodology, instrumental costs are intentionally omitted from the equation. While these costs, encompassing the expenses related to equipment and machinery, undoubtedly contribute to the overall expenditure, their exclusion allows us to present a focused and simplified perspective. This deliberate choice enhances clarity and facilitates a more accessible understanding of the primary cost drivers. In summary, our approach aims to empower decision-makers with a clear and comprehensive view of the financial landscape associated with material production. By delineating the costs of raw materials, utilities, and labour, we provide a foundational understanding that can guide efforts to optimize material compositions and production processes for enhanced economic viability and industrial applicability.

We follow these steps to find the annual energy consumption of a product, as well as the cost to operate it [36]. We use certain generic formulae, which we have provided below with references, to calculate energy usage and energy footprint. We must estimate how many hours per day an appliance runs and determine the machine's wattage to compute this. The energy footprint of our product is then determined by adding the value to the calculation.

1. Daily Kilowatt − hr (kWh)consumption $= \frac{\text{Wattage X Hrs Used Per Day}}{1000}$.
2. The annual energy consumption $=$
   Daily kWh consumption X number of days used per year.
3. The annual cost to run the appliance $=$
   Annual energy consumption X utility rate per kWh.

This is one of the straightforward formulas we use to estimate the cost of electricity for each step of the synthesis process for our products.

3. Precursors to MAX phase

For the synthesis of MXene, this is the first step after selecting the precursors. Ball milling machines and tube furnaces, among other equipment, will be used throughout these processes. Variables such as temperature, heating, and reaction time play a pivotal role. Fig. 3 depicts the processing flow from the precursor to the MAX phase. A closer look reveals that the processes in question are associated with precursors, ball milling, tube furnace, and grinding. All the steps are equally necessary for synthesis, although tube furnaces play a disproportionately large role in the process. Both the variables and utilities directly involved in increasing or decreasing the value of MXene are also demonstrated in Fig. 3. These factors are crucial for the production of MXene and are strongly correlated with the cost of MXene in the long run.

The synthesis of the MAX phase requires a particular range of temperatures. However, it is necessary to analyze the optimum temperature to synthesize the MAX phase efficiently. An unnecessary increment of the temperature results in energy waste, whereas a substantially lower temperature leads to the unfeasibility of synthesizing the MAX phase. As with this, it is necessary to increase the temperature by using some grading. If the grading is not appropriate, then the tube furnace needs to run for a long time for operation, resulting in additional burning of gas and electricity. The same is true for holding time. If it is kept for a longer holding time, then all utilities would increase the cost of the final product. The first process is needed for a ball milling machine, and the

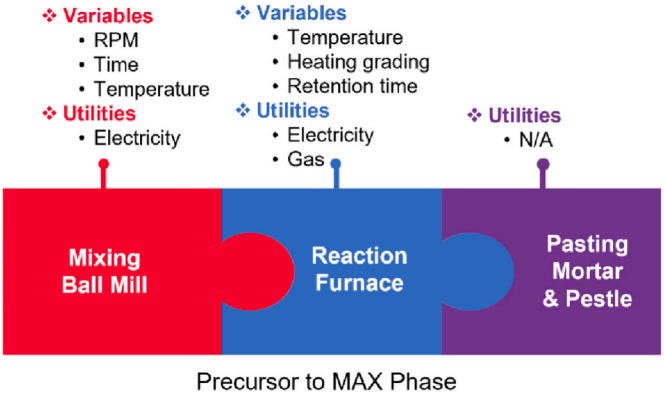

Fig. 3. Processing steps in converting the precursors to MAX phase with the involved variables and utilities that impact the production cost of MXene.

second is a tube furnace. The approximate time of the first process is 17–24 h but it depends on the precursors, process, and many other things [37]. In a ball mill, the only consumable item is electricity, and in a tube furnace, the utilities are gas flow to protect from oxidation and electricity. Following this procedure, MAX phase components will have a brick- and light-grey appearance. Etching produces a powdered form of the MAX phase. Etching is to remove the 'A' element during the chemical etching process. That process forms the MXene by using MAX phase materials.

3.1. Precursor selection

Precursor selection is a critical step in the synthesis of MXene. Most studies use Ti, Al, and C as precursors. The precursor selection depends on the application, cost, and other factors. Some of the precursors, such as Zr, are less expensive than others. Aside from the cost of the materials, the molar ratio adjustment is also an essential part of making MXene. In this study, we provide some potential and developed precursors and the precursor ratios that researchers have previously utilized to synthesize MXene effectively. However, in most circumstances, $Ti_3C_2T_x$ takes precedence [38]. As a result, this type of MXene is used to calculate the synthesis cost per 1 g in this work. According to our calculations, considering the MXene precursor ratio, the cost of our precursors for 100 g is $ 420.23 in 2022. This indicates that 1 g is worth only $ 4.20.

3.2. Ball milling

The controlling parameters for the ball milling process are speed, operating time, and ball size. Ball mills are used to grind materials down to a finer consistency and achieve a uniform combination of all ingredients [39]. Some researchers have shown that the reaction temperature of materials in a ball mill within a jar can be very high and affect the yield [40]. However, this is not our primary focus. Cost estimation is a significant issue for us and is directly related to how long this ball milling machine is used. An electric ball mill used here at the facility requires 2.8 kWh to run. In our case, the precursors undergo a ball milling process for 4 h and maintain a speed of 400 rpm, the cost per unit of energy is $0.081, and the maximum capacity of the ball milling jar is 250 g. Therefore, the cost per gram of mass produced by this machine is readily calculable using equation (1).

$$\text{Ball milling cost} = \left[\frac{\textit{Electricity consumption} \times \textit{Running time} \times \textit{Electricity cost per unit}}{\textit{capacity of the machine}}\right] \quad (1)$$

For our case, the electricity consumption is 2.8 kWh, and the machine operates for 4 h while the capacity of the ball milling machine is 250 g. Considering the cost per unit of electricity as $0.081, the ball milling cost can be found as $0.010.

3.3. Tube furnace

The tube furnace is crucial to the MXene synthesis process [41]. When working with a tube furnace, the materials must be kept in a vacuum chamber or closed chamber, which must then be purged with argon (Ar) gas [42]. Researchers have proposed using carbon dioxide (CO_2) or nitrogen gas (N) to eliminate oxygen (O_2) precursors and protect against tube contamination. However, a rapid temperature rise may not be conducive to all processes. However, if the temperature is raised gradually, the process takes longer, uses more power, and raises the cost of MXene. To conduct the experiment, we must prepare the experimental heating grade. In the synthesis of the MAX phase from precursors investigated by prior researchers, a tube furnace is utilized for its enhanced safety features, ensuring a controlled internal environment crucial for the high-quality production of the MAX phase and subsequently, MXene. Our tube furnace can hold up to 150 g of precursors. This tube furnace has a 7 h cycle time and uses just 0.1 kWh of electricity. The cost of operating the tube furnace can be determined using equation (2).

$$\text{Furnace cost} = \left[\frac{\textit{Electricity consumption} \times \textit{Running time} \times \textit{Electricity cost per unit}}{\textit{capacity of the machine}}\right] + \textit{Gas cost} \quad (2)$$

Considering the cost of gas as $ 3.66. the furnace cost can be calculated as $ 3.6603, which indicates that the cost of gas is the key determining factor for the furnace cost.

Table 1 shows the costs of various MAX phase materials, based on the prices of different elements. It is evident from the table that Ti_3AlC_2 is the second most affordable MAX phase material. Additionally, using carbon instead of graphite for MAX phase synthesis proves to be a cost-effective approach, as graphite is one of the sources of carbon for MAX phase synthesis. Hence, this table provides researchers with a comprehensive understanding, enabling them to make informed decisions when selecting the most economically viable MAX phase or MXene for synthesis.

3.4. Grinding

Samples of the so-called MAX phase often seem like a small brick or light ash after being extracted. However, this might vary depending on the precursors employed to synthesize the MAX phase and the quality of the materials' hardness. So, we need to grind the etching ingredients into a powder [56]. Researchers recommend using a drill bit to break down MAX phase materials at these stages but doing so requires energy and might drive up the cost of the MAX phase components. Therefore, a hand mortar and chalk for making powder are recommended for these procedures. Since it does not need any infrastructure, like electricity, it leaves no economic trace.

In our analysis, we do not factor in the use of a drill to produce powder from MAX phase material for etching. The MAX phase powder is made by using a manual mortar and pestle; thus, no power is needed for this process. Therefore, there is no financial outlay associated with this action. This step has no cost allocation as this is a laboratory-scale cost analysis. However, on a large scale, this step would incur some costs.

4. MAX phase to Mxene

MXene is synthesized in two stages, as was mentioned before. The conversion of the MAX phase to MXene is the second and most crucial step in the MXene production process. A magnetic hot plate stirrer and laboratory apparatus chemically compatible with HF, together with known techniques for the synthesis of MXene, are required for this procedure; They are described in detail in Table 2. While there are several well-established routes for MXene production [37], the MAX phase materials etching with hydrofluoric acid is the focus of this research work. LiF and HCl (high concentration) are required for this procedure. The primary controllable parameters of this procedure are the reaction temperature, the reaction time, and the stirring speed. As

Table 1
Precursors used for synthesizing the MXene with a ratio of precursor and price of the individual's precursors collected from Sigma Aldrich.

SL	AL	Ratio	Amount (g)	P-1	Price (USD)	P-2	Price (USD)	P-3	Price (USD)	100g/USD	Ref.
1	Zr_2AlC	2:0.8:1.2	100	Zr_2	760.76	Al	4.54	C	30.83	796.13	[43]
2	Ti_3AlC_2	3:1.2:1.8	100	Ti	338.69	Al	4.54	C	77	420.23	[44,45]
3	Ta_3AlC_2	3:1.2:1.8	100	Ta	409.2	Al	4.54	Graphite	77	490.74	[46]
4	Zr_3AlC_2	3:1.2:1.8	100	ZrH_2	171	Al	4.54	Graphite	77	252.54	[47]
5	HF_3AlC_2	3:1.01:1.8	100	HF	1056.34	Al	3.94	Graphite	79.6	1139.88	[48]
6	$Ti_5Al_2C_3$	5:2.15:2.78	100	Ti	341.06	Al	4.91	Graphite	69.59	415.56	[49]
7	Ti_4AlN_3	50:13.5:36.5	100	TiH_2	114.29	Tin	34.96	AlN	60.7	209.95	[50]
8	Ta_4AlC_3	4:1.25:2.6	100	Ta	450.39	Al	3.61	Graphite	84.94	538.94	[51]
9	Nb_4AlC_3	2:1.2:0.9	100	Nb	246.82	Al	6.439	Graphite	56.19	309.449	[52]
10	V_4AlC_3	4:1:3	100	V_4	870.1	Al	2.75	Graphite	96	968.85	[52]
11	Mn_2GaC	2:1:1	100	Mn	214	Ga	330	Graphite	64	608	[53]
12	Ti_3GaC_2	2.1:2.3:1.7	100	Ti	233.06	Ga	497.7	Graphite	71.34	802.1	[54]
13	Nb_2GeC	2:1:1	100	Nb	253	Ge	763.25	Graphite	64	1080.25	[55]
14	Ti_2InC	2.1:2.3:1.7	100	Ti	233.06	In	640.22	Graphite	71.34	944.62	[54]

Table 2
Different types of methods for synthesizing the MXene.

SL	Name of the methods	References
1	Hydrofluoric Acid Etching	[59]
2	Fluoride Salt Etching	[60]
3	Fluoride-Free Etching	[61]
4	Electrochemical Etching Method	[62]
5	Molten Salt Etching	[63]
6	Chemical Vapor Deposition (CVD)	[64]

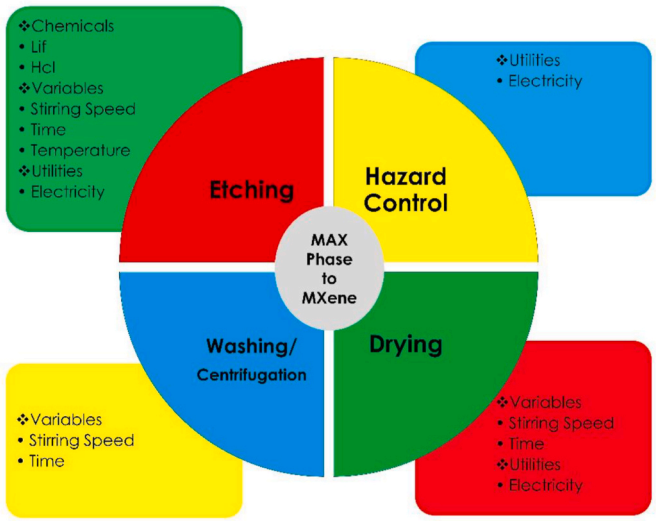

Fig. 4. Process involves the MAX phase to MXene with the variables and utilities impacting the price of the MXene.

the reaction is exothermic and emits smoke that is harmful to human health, precautions must be taken to prevent any potential damage [57,58].

The production of MXene from the MAX phase with the involved processing steps is shown in Fig. 4. The processing steps involve etching, hazard control, washing, centrifugation, and drying. Although all of them are necessary for a successful synthesis, etching and centrifugation are particularly crucial. The utilities and influencing factors that directly impact the MXene's monetary worth are also mentioned in Fig. 4.

4.1. Etching

Our research has shown that the essential steps in synthesizing MXene are determining how much acidic solution to make and then precisely adding the MAX phase components to the reaction bottle. The use of heat and constant stirring will speed up the process [65]. These components increase production costs since they need the power to operate. Time is also a significant factor. The whole reaction will take approximately 12–24 h to occur. Some researchers claimed they could produce MXene in 6–12 h in the lab [66]. Although the time required varies with the quality of the yield, our research suggests that it takes at least 12 h. To determine how much the etching procedure will cost, we need to consider the operating time, electricity consumption, and the chemicals that are used for the etching process. The etching cost can be calculated by using equation (3).

$$\text{Etching cost} = \left(Cost\ of \frac{HCl}{ml} \times Required\ ml\ of\ HCl\right) + \left(Cost\ of \frac{LiF}{g} \times Required\ gram\ of\ LiF\right) \quad (3)$$

The required amount of HCl and LiF is 15 ml and 1.6 g [67], which cost $ 0.16 per ml and $ 0.83 per g, respectively. Therefore, the cost for etching can be calculated as $ 3.18.

4.2. Stirring and heating

While the etching process is in progress, it is necessary to aid the etching process by providing heat and stirring the solution. To do this, a magnetic hot plate stirrer and a magnetic bar are usually used to keep the solution well mixed and increase the temperature. To produce heat and a magnetic field, the hot plate requires electricity [57]. Because of the prolonged duration of the process, the only relevant resource is electricity consumption, which must be calculated. The cost for stirring and heating can be found by using equation (4).

$$\text{Stirring and heating cost} = \left[\frac{Electricity\ Consumption \times Time \times Electricity\ cost\ per\ unit}{capacity\ of\ the\ machine}\right] \quad (4)$$

For a 150 g capacity machine that consumes 0.65 units of electricity for 24 h of operation at an electricity cost of $ 0.081 per unit, the cost for

stirring and heating can be found at $ 0.008.

4.3. Hazard control

The etching reaction is exothermic, and the chemicals involved are corrosive owing to their chemical composition [41]. Carcinogenic HCl vapers were constantly present during the process. We must use fume hoods and protective masks to keep ourselves safe throughout the reaction [26]. However, electricity is a must for operating the fume hood, and the synthesis cost goes up. Although the price is modest, it must be included to obtain a more accurate cost. Equation (5) can be used to find out the cost associated with hazard control.

$$\text{Cost for hazard control} = \left[\frac{\textit{Electricity Consumption} \times \textit{Time} \times \textit{Electricity cost per unit}}{\textit{capacity of the machine}}\right] \quad (5)$$

Considering the flame hood's running time of 24 h which consumes 0.65 units of electricity, the cost for hazard control can be estimated at $ 0.008.

4.4. Washing and centrifugation

When acid is used to etch materials, the pH of the reaction medium decreases. The pH level of the materials must be adjusted to between 6.7 and 7 by repeated washings. The materials will be cleaned and brought to the proper pH level, which also requires the use of an ultra-high-speed centrifuge to separate the materials from the water. With the water being used during the washing process, it is considered a by-product. Because of the pollution and low pH level, this water poses risks to human and environmental health [68]. To protect ourselves from inhaling the poisonous vapours produced during the washing process, we must use the proper respirator mask before beginning the wash. We need to purge the material of contaminants (excessive salts and unetched MAX phase from the sample) before obtaining single and multi-layer MXene. Although single layers are not inherently impure, they are preferred in certain situations, including electrochemical applications [69]. The ultra-high-speed centrifuge is powered by electricity, and its operation duration varies with the complexity of the procedure and level of expertise. If the stirring speed is too slow, the MXene dispersion cannot be separated from the water and made dry. However, if it has been left on for too long, it consumes more power, and the structures are also damaged [70]. It might end up influencing the retail price. The typical operating speed is 3500–4500 rpm, with a running period of 5–7 min. The associated cost can be calculated from equation (6).

$$\text{Washing or centrifugation cost} = \left[\frac{\textit{Electricity Consumption} \times \textit{Time} \times \textit{Electricity cost per unit}}{\textit{capacity of the machine}}\right] \quad (6)$$

For a 60 g capacity machine that consumes 4.53 kWh of electricity at a unit cost of $ 0.081 and runs for 1.5 h, the cost can be estimated at $ 0.009.

4.5. Drying

When the material's pH is between 6 and 7, it is removed from the water and dried in a petri dish inside a vacuum oven. To prevent the product from being contaminated while drying due to oxidation, we must put it in a vacuum. MXene, for whatever reason, does poorly in the presence of oxygen [46]. A review of the available literature suggests that MXene's characteristics diminish when exposed to oxygen. However, it is still unclear exactly how MXene degrades in an aquatic environment [71]. This issue is not covered in depth in this paper, but we concentrate on the preventative measures that may result in higher synthesizing costs for MXene. The cost of drying can be calculated from equation (7).

$$\text{Drying cost} = \left[\frac{\textit{Electricity Consumption} \times \textit{Time} \times \textit{Electricity cost per unit}}{\textit{capacity of the machine}}\right] \quad (7)$$

A 150 g capacity drying machine that consumes 0.1 kWh of electricity and runs for 12 h during the drying process will cost $ 0.00064, considering that the cost per unit of electricity is $ 0.081.

5. Storage condition

We need to keep the as-prepared materials for an extended duration; thus, the storage environment is essential. Instead of using a conventional refrigerator, which uses energy, a common desiccator should be utilized. In addition, preventing the MXene from oxidizing is crucial. Maintaining a dry environment in the desiccator with the help of an appropriate drying agent keeps the sample from coming into contact with moisture and decreases the risk of oxidation. Additionally, the absence of oxygen in a vacuum setting slows the oxidation process. A vacuum desiccator is used to prevent the oxidation of the materials [72]. Desiccators, with or without argon gas, are used to store samples. To keep costs down, we are not using argon gas. Other researchers have proposed keeping MXene as a liquid, but we think it would be far more convenient and much better to keep it as a powder.

6. Characterization

Characterizations are needed to verify the practical synthesis of MXene, adding an indirect cost to the overall manufacturing of this emerging nanomaterial. The morphological and structural characteristics of MXene are easily exposed and observed using an imaging method like the SEM and TEM. Tungsten filaments in airtight environments

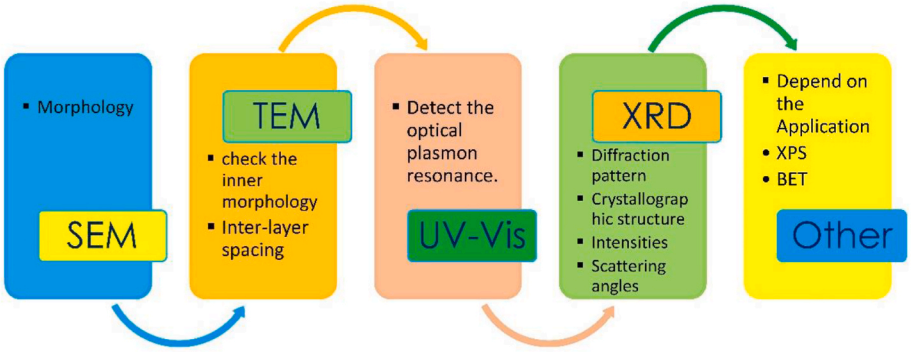

Fig. 5. Flow diagram of MXene for various characterization purposes by using different types of instruments.

Table 3
Cost associated with the characterization of MXene.

Description	Cost in RM	Cost in USD (As per conversion rate in May 2023)
SEM (Scanning Electron Microscope)	150	33
FESEM (Field emission scanning electron microscopy)	400	88
XRD (X-ray diffraction analysis)	200	44
XPS (X-ray photoelectron spectroscopy)	350	77
UV–Vis (Ultraviolet–visible spectroscopy)	100	22

generate electron beams in TEMs. The electrons are accelerated and focused by an electromagnetic field. The beam then penetrates a sample with a thickness of less than 100 nm. When electrons are sent through the sample, an image is formed on a phosphor screen, CCD, or film. By decreasing the sample density, more electrons may pass through, improving the image's contrast. A decrease in electron transmission caused by a denser sample yields a darker final image [73]. In addition to SEM and TEM, MXene's plasmon resonance allows UV–Vis spectroscopy to characterize their optical property by identifying their plasmon absorbance peak at a specific wavelength range [74].

The last and most essential test is XRD analysis, which is a method used in materials science to identify a material's crystallographic structure. The XRD technique involves exposing a sample to incoming x-rays and then measuring the emitted x-rays' intensity and scattering angle. Ti_3AlC_2, Ti_2AlC, and Ti_3SiC_2 are all examples of MAX phases that XRD can identify; this test is not difficult to perform, but it needs a high-tech XRD apparatus. Thus, it is not cheap. Different types of MAX phases could be detected by XRD, allowing for an assessment of the MAX phase's quality. To ensure high-quality MXene is synthesized, this fast, non-invasive, non-destructive, and easy technique performs phase identification via crystallographic analysis to confirm the success of the synthesis of MAX and MXene [73]. Fig. 5 depicts the flow of MXene's characterization processes. SEM, TEM, UV–Vis, and XRD are the processes involved in the characterization process. All of the processes are vital to synthesis, but XRD is the most significant. We also illustrate the factors and particular studies that are directly engaged in boosting or reducing the financial worth of the MXene in Fig. 5.

All the characterization processes are crucial to the analysis, and most of the time, the testing equipment is expensive to run due to expenses associated with consumable materials or components, maintenance, and calibration charges. In such an instance, calculating the cost based on the characterization methodologies is problematic. This component, however, cannot be overlooked since the confirmation of MXene production is entirely reliant on it. Analytical methods such as XRD, UV–Vis, SEM, and others provide scientific proof before the MXenes are used in specific applications or integrated with other materials. Other related methods such as Brunauer-Emmett-Teller (BET), x-ray photo electron spectroscopy (XPS), Raman spectroscopy, and so on are also significant, but only if the quality in terms of specific qualities is critical for use in applications such as energy storage, electrocatalysts, water treatments, optoelectronics, and so on. The strategies mentioned above solely depend on the investigation's primary goal. The essential analytical procedures shown in Fig. 5 are only considered to constitute a fraction of the synthesizing cost in this research. We gathered various commercial quotas for characterization testing to validate and assess the cost estimate. All commercial quotations are collected in Malaysian currency and translated to USD, which is presented in Table 3. We conduct the necessary and essential characterizations on every batch of the produced MXene for quality assurance and consistency. In this case, we only consider the cost of SEM, XRD, and UV–Vis in the synthesis cost of MXene.

7. Human effort expense

One of the essential factors in determining the cost of MXene is the cost of human effort. We attempted to convey that the human effort cost is determined using the cost of a research assistant (RA) based in the Malaysian area. An RA's monthly pay in Malaysia is around (Ringgit

Table 4
Estimation of the processing time of every single step of MXene synthesis.

SL	Description	Time
01	Sample Preparation (Precursors measuring)	1 h.
02	Ball Mill	3 h.
03	Tube furnace	7 h.
04	Grinding	1 h.
05	Etching Process	24 h.
06	Washing	2 h.
07	Drying	8 h.
08	Storage	1 h.
09	Other	1 h.

Table 5
Cost calculation of the MXene.

SL	Cost components	Cost per gram (USD)
1	Precursors	4.20
2	Ball millings	0.010
3	Thermal treatment	3.66
4	Grinding	0
5	Etching	3.18
6	Stirring	0.008
7	Hazard control	0.008
8	Washing	0.009
9	Drying	0.0006
10	Characterization	0.820
11	Human effort expense	0.305
Total Cost		**$ 12.20 (USD)**

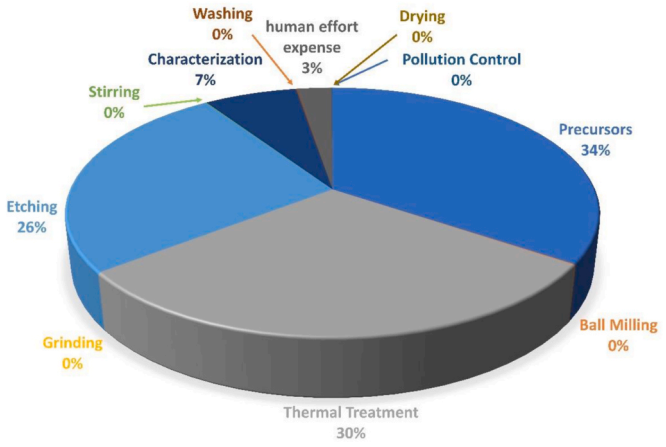

Fig. 6. Economic footprint of different steps in MXene synthesis.

Malaysia) RM 2500, which is equivalent to $ 550. Then, to evaluate the economic impact of the MXene synthesis, we must determine the cost per hour. The RM 2500 monthly compensation is translated to an hr/daily rate in this scenario.

Table 4 presents the detailed time estimation of every single step of the MAX and MXene synthesis process. This time should be varied due to the etching method, different precursors, and the different types of MXene. We must determine how much assistance time is needed for MXene production. We need 48 h (2 days) of assistance for our concept's whole synthesis process of MXene. Human effort is needed for the steps of Ball mill loading, furnace loading, MAX phase takeout from the furnace, making powder using a mortar pestle, initiating the etching process, washing the sample after etching, loading the oven, takeout the sample from the sample from oven, and storage the materials. We consider these 48 h (2 days) to be the only work for production MXene. The machine then completes the remaining tasks on its own (e.g., when MAX phase powder is already added to the solution, it is just left to complete the reaction/etching process after that takeout the solution and wash it). If we multiply by daily pay, the total cost of human work is $ 0.093 per g of MXene. The cost can be realized by using equation (6).

$$\text{Human effort expense} = \frac{\frac{\text{Wage of RA}}{\text{Working days in a month}}}{\text{working hours in a day}} X \; Hours \; of \; Assistance \; needed \; / \; amount \; of \; MXene \; produce \; of \tag{6}$$

The cost associated with the human effort resulted in $ 0.305.

8. Final cost calculation

After adding all the cost components, the final cost is calculated, which is presented in Table 5.

In our meticulous cost analysis, we account for every individual cost associated with the synthesis of MAX phase materials used in the production of MXene. After considering all components, the calculated final cost stands at $ 12.20/g for the MAX phase materials. However, it's crucial to introduce a critical factor into this assessment—yield. When we transition from the precursor MAX phase materials to the final product, MXene, we encounter a yield of 60 % [75]. This means that from the initial 1 g of MAX phase materials, we obtain 0.6 g of MXene. Now, shifting our focus to this pivotal point, the recalculated cost of 1 g of MXene becomes $ 20.33. This adjusted figure considers the efficiency of the synthesis process, providing a more accurate representation of the cost per gram for the final product. This nuanced perspective, factoring in yield, offers a clearer and more realistic understanding of the economic considerations associated with MXene production. It underscores the importance of not only considering raw material costs but also acknowledging the efficiency of the synthesis process in determining the ultimate cost of the product.

9. Economic footprint in different steps

The cost of MXene in Malaysia has been effectively approximated. The pie chart in Fig. 6 shows the breakdown analysis for the separate costs associated with all of the preparatory procedures involved in the synthesis of MXene. It depicts the economic footprint based on the different synthesis phases, characterization, and human effort expenditures. There are eleven phases involved in the synthesis process; where the most important contribution is the choice of precursors, which occupies 34 % of the overall cost, and the second one is a thermal treatment or tube furnace. This step has a 30 % impact. The next most expensive phase is an etching, which is 26 %. So, if cost reduction is essential for the commercialization of MXene, we must keep an eye on these steps.

However, some other steps are less significant in terms of cost, but they are just as vital since all the various steps are interrelated to ensure the production and quality of the MXene. If any procedures are not followed correctly, the ultimate product will be impeded and fail, resulting in financial and time losses.

10. Conclusions

To summarize, we provide a comprehensive overview of the MXene synthesis procedures, accompanied by specific guidelines during the synthesis process. We meticulously identify the cost components and factor in their associated expenses to calculate the cost per gram of MXene. The overall cost of producing 1 g of MXene is determined by incorporating the costs associated with various stages of synthesis, characterization, and labour. Commercial quotations are employed to assess the cost of characterization, while the expenses related to equipment and infrastructure are excluded from our computations. The final cost of synthesizing 1 g of MXene is evaluated at $ 20.33. Furthermore, our detailed analysis incorporates precursor prices, equipping researchers with a thorough comprehension to facilitate informed decisions in the selection of economically feasible MAX phase or MXene materials for synthesis. Each step of the individual calculation serves as a guideline to minimize the cost of MXene, a crucial stride towards the commercialization of these emerging materials. We anticipate substantial benefits for the scientific community through this study, aiding researchers in the systematic organization of their work and optimization of the synthesis process.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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