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Citation for the original published paper (version of record):
Furberg, A., Arvidsson, R. (2024). Life Cycle Assessment of Synthetic Nanodiamond and Diamond Film Production. ACS Sustainable Chemistry & Engineering, 12(1): 365-374.
http://dx.doi.org/10.1021/acssuschemeng.3c05854

ACS Sustainable Chemistry & Engineering
pubs.acs.org/journal/ascecg
Research Article

Life Cycle Assessment of Synthetic Nanodiamond and Diamond Film Production

Anna Furberg* and Rickard Arvidsson

Cite This: ACS Sustainable Chem. Eng. 2024, 12, 365−374
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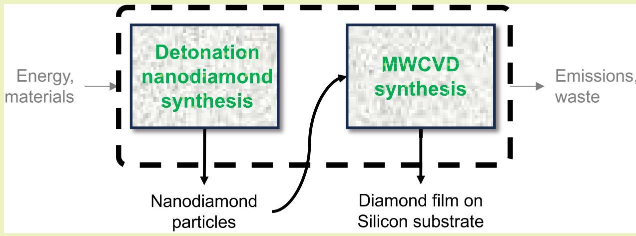
ABSTRACT: Diamond possesses extraordinary properties, including extreme hardness, thermal conductivity, and mechanical strength. Global industrial diamond production is dominated by synthetic diamond, with important commercial applications in hard coatings and semiconductors. However, the life cycle impacts of synthetic diamond materials are largely unknown. The main aim of this study is to conduct the first detailed life cycle assessments of the typical production routes for nanodiamond and diamond film, which are detonation synthesis and microwave chemical vapor deposition, respectively. The functional units were set to 1 g nanodiamond and 1 cm^2 diamond film. A limited number of inputs dominate the assessed impacts: explosives and cooling water for nanodiamond production, and electricity and substrate for diamond film production. Diamond film manufacturers can reduce their global warming, freshwater eutrophication, and terrestrial acidification impacts by 62−71% by sourcing wind or solar instead of global average electricity. However, this comes at the expense of increased mineral resource scarcity impacts at 57−73%. A comparison between nanodiamond and synthetic diamond grit shows that the grit's global warming impact is about 5 times higher, suggesting that nanodiamond is environmentally preferable. The ready-to-use unit-process data from this study can be applied in future studies of products containing these materials.



KEYWORDS: *detonation nanodiamond, diamond film, detonation synthesis, microwave chemical vapor deposition, life cycle assessment, life cycle inventory*

INTRODUCTION

The outstanding properties of diamond put it among the top advanced materials whose development might lead to major scientific breakthroughs in the 21st century.[1] In 2022, more than 3000 metric tonnes of industrial diamond was produced globally.[2] About 99% of this was synthetic diamond, with China, the United States, and Russia as the top 3 producing countries, and the remaining 1% was natural diamond. Synthetic diamond production is now a mature technology,[1] and research is ongoing to improve existing production technologies as well as develop novel ones. The most common technologies for industrial synthetic diamond production are high-pressure high-temperature (HPHT) synthesis, chemical vapor deposition (CVD),[1,3] and detonation synthesis.[4] Among CVD technologies, microwave chemical vapor deposition (MWCVD) is most widely applied.[3] These production technologies generate different types of synthetic diamond materials, ranging from large single-crystal diamonds and diamond grit to diamond films and nanodiamonds (Figure 1). Some of these production technologies are also interconnected, for example, nanodiamonds are typically added as seeds in diamond film production.[1]

Synthetic diamond materials have both commercial and promising future applications. Nanodiamonds, with a crystal size of <100 nm,[5] are currently used in, e.g., finish polishing and metal-nanodiamond coatings due to their high hardness, thermal conductivity, and mechanical strength.[4,6] Recently, nanodiamonds have also gained attention for their potential use in thin-film electronics, photovoltaic devices, and energy storage devices, where properties such as high stability and thermal conductivity are required.[4] Diamond films are mono- or polycrystalline layers that can be produced in both thin (<100 μm) and thick (>100 μm, <1 mm) sizes.[1] Today, diamond films are used as, e.g., semiconductors due to their wide band gap and high thermal conductivity and coatings on cutting tools, due to their extreme hardness and high wear resistance.[7] Additional promising applications of nanodiamonds and diamond films under fast development include quantum photonics and quantum computers.[8] In fact, nanodiamond is expected to be the second-most used specialty nanomaterial within a decade.[9]

Considering the ongoing developments of existing and novel synthetic diamond production technologies, it is important

Received: September 12, 2023
Revised: December 8, 2023
Accepted: December 11, 2023
Published: December 20, 2023

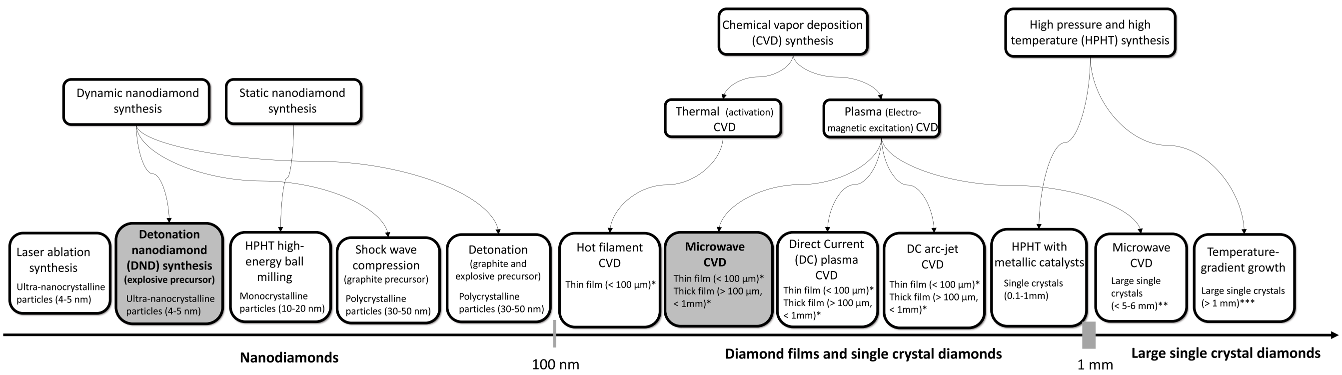


Figure 1. Overview of commercial synthetic diamond types and their production technologies. Detonation nanodiamond (DND) synthesis and microwave chemical vapor deposition (MWCVD) are assessed in this paper and therefore highlighted in gray. The figure was developed based on Kumar et al.[4] and Shenderova and Nunn[5] for nanodiamonds and Palyanov et al.[1] and Varnin et al.[21] for diamond films, single-crystal diamonds, and large single-crystal diamonds. * Requires a diamond substrate (natural or high-pressure high-temperature (HPHT) diamond) or diamond seeds (nanodiamonds) when a nondiamond substrate is used. ** Requires a large single-crystal diamond seed. *** Requires diamond seeds acting as the carbon source (single-crystal diamonds) and a diamond seed (large single-crystal diamond).

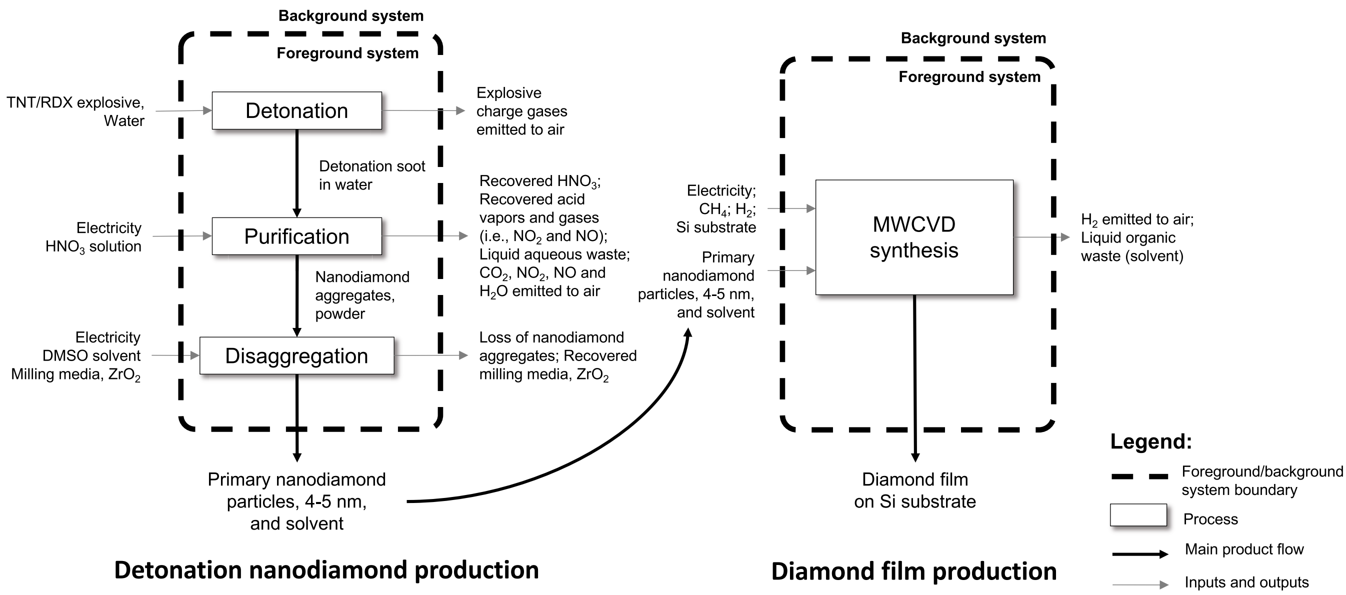


Figure 2. Flowchart for the interconnected technologies of nanodiamond production via detonation and diamond film production via microwave chemical vapor deposition (MWCVD). CH_4 = methane; CO_2 = carbon dioxide; DMSO = dimethyl sulfoxide; H_2 = hydrogen. H_2O = water; HNO_3 = nitric acid; NO = nitrogen oxide; NO_2 = nitrogen dioxide; RDX = 1,3,5-trinitroperhydro-1,3,5-triazine; Si = silicon; TNT = 2,4,6-trinitrotoluene; ZrO_2 = zirconium dioxide.

that their environmental impacts are minimized. Kumar et al.[4] stated that the development of nanodiamond synthesis processes with lower environmental impacts is critical. Life cycle assessment (LCA) is commonly applied to assess environmental impacts over the life cycle of products, from raw material extraction to the end of life.[10] Until now, however, the life cycle impacts of synthetic diamond materials have only been investigated to a limited extent. The conventional diamond grit production via HPHT synthesis has been assessed by Furberg et al.[11] Some life cycle environmental data were provided by Ferreira et al.[12] for an alloy containing detonation nanodiamonds (DNDs), but no data on nanodiamond production was provided. Wilfong et al.[13] provided LCA results for synthetic diamond film production by hot filament CVD synthesis at laboratory scale. Some studies assessed wastewater treatment technologies with boron-doped diamond electrodes by upscaling of laboratory data.[14,15] The CVD technology considered in these studies was not stated, although the data sources in Surra et al.[15] indicated that at least some of their unit-process data represented hot filament CVD. To the best knowledge of the authors, no LCA has been performed for DNDs and diamond film from MWCVD.

To address this gap, the aims of this study are to (i) provide detailed LCA results for DND and diamond film from MWCVD, and (ii) provide recommendations toward reduced impacts. The intended applications of the results are by LCA practitioners in future studies of products containing these materials and to guide synthetic diamond manufacturers toward reducing environmental impacts. This study furthermore contributes to the body of knowledge on the life cycle impacts of carbon-based nanomaterials.[16−20]

■ MATERIALS AND METHODS

An attributional LCA, which considers impacts of environmentally relevant physical flows to and from the product system,[22] was conducted for DND and diamond film. The system boundary is cradle to gate, including raw material extraction and the production of the product.[23] Cradle-to-gate studies can be conducted as a first step to assess the environmental impacts of materials and provide important input data to cradle-to-grave studies.

Functional Unit. The functional unit constitutes a quantitative reference to which the environmental impacts are related and should reflect the function of the product assessed.[23] In cradle-to-gate studies, with the aim to assess the environmental impacts of a single product, the functional unit might be set equal to a physical output, such as mass.[24] Although a mass-based functional unit does not reflect material properties or functions, it can still be relevant in studies with the aim to conduct approximate comparisons of materials' environmental impacts if these are used in similar applications, particularly for novel materials.[25] A mass-based functional unit of 1 g nanodiamonds (4−5 nm primary particles) was selected for detonation synthesis. The particle size and shape influence nanodiamond properties and are selected based on the intended application.[4] DNDs, with typical particle sizes at 4−5 nm,[5] are advantageous in, e.g., abrasive treatment of superhard materials due to the resulting low surface roughness.[6] The particle size depends on the synthesis method applied;[4] see Figure 1 for an overview of common nanodiamond production technologies and the corresponding particle sizes. The exact DND composition and purity commonly varies between vendors depending on synthesis and purification conditions.[26]

For the production of diamond film via MWCVD, a functional unit of 1 cm^2 diamond film with a 10 μm thickness, corresponding to 3.2 mg diamond film with a density of about 3200 kg/m^3,[27] was selected. A thickness of 10 μm was selected as this is a common order-of-magnitude thickness for diamond films.[28] In addition to this, information on how to obtain results for diamond film of other thicknesses is provided in Section S3.1 in the Supporting Information (SI). Diamond film properties can be steered and tailored for specific applications via growth process parameters, such as temperature and pressure, in turn dependent on, e.g., the CVD apparatus power.[27] Furthermore, MWCVD allows for growing the purest optical- and electronic-grade diamond since the film is not contaminated by electrode sputtering products as for other CVD methods.[1]

Systems Studied. The systems assessed are shown in Figure 2 and are interconnected because DND is an input material to the diamond film production. Both synthetic nanodiamonds and diamond films are currently produced commercially.[1,6] Data representing industrial-scale DND and diamond film production were collected for the foreground system, i.e., the part of the system within the influence of producers, representing the highest technology readiness level (TRL) of 9.[29] Flows related to personnel and capital goods are not included in the foreground system data. The foreground system data are provided in the Calculations section. The background system is not under direct influence of the producers, so changes can only be realized through indirect actions, such as sustainable procurement. The background system was modeled with generic data, see the Background System Data section. The cutoff approach was applied to allocate impacts between processes shared by different product systems, which means that burdens directly caused by a product are assigned to that product.[30]

Life Cycle Impact Assessment (LCIA). The life cycle impact assessment (LCIA) method ReCiPe 2016 midpoint v1.1 with the hierarchist perspective[31] was applied to quantify environmental impacts. The four impact categories global warming, freshwater eutrophication, terrestrial acidification, and mineral resource scarcity were selected to be in focus and are described in Section S5 in the SI. These impact categories are commonly applied in previous LCAs of synthetic diamond, see, e.g., Ferreira et al.,[12] Sun et al.[14] and Furberg et al.,[11] and were selected to represent both environmental and resource impacts. In addition, results for all impact categories in the ReCiPe 2016 midpoint method are provided in the SI. The open-source software OpenLCA v1.10.3 (GreenDelta) was applied for the LCIA calculations.

Background System Data. Background system data were chosen to represent global average production and were mainly obtained from the Ecoinvent database v.3.7[32] with the "allocation, cut-off by classification" system model. When data representing global production were unavailable, data representing the "rest of the world" (i.e., average data for nonspecified geographical locations) were selected instead. In some cases when data were unavailable in the database, literature sources were utilized instead: Data on explosives used in DND production were obtained from Häggvall et al.[33] and Ferreira.[34] The background system data applied are listed in Section S6 in the SI.

Uncertainty and Sensitivity Analysis. Model uncertainties were assessed via scenario analysis.[35] A baseline scenario was constructed, representing global industrial production of DND and diamond film. In addition, three alternative scenarios were constructed to assess how changes in the product systems would influence the impacts. In the first alternative scenario, the global average electricity input to the foreground system was replaced by an optimistic scenario based on a renewable, flow-type energy source with low emission intensity, modeled with pure wind power as proxy (ca. 34 g CO_2 equiv/kWh). In the second alternative scenario, solar power was applied as proxy instead (ca. 73 g CO_2 equiv/kWh). These alternative scenarios represent cases in which the synthetic diamond producer decides to source decarbonized electricity through green tariffs. In the third alternative scenario, the solvent dimethyl sulfoxide (DMSO) was replaced by deionized water, representing the case where the DND producer decides to change the type of solvent applied. An overview of the scenarios is provided in Table S9 in the SI.

Parameter uncertainty was assessed through a sensitivity analysis by altering the value of each parameter at a time to see how this affected the results. When data ranges were available, the average value was applied in the baseline scenario, while the lower and upper values were considered in the sensitivity analysis. If only one value was available, that value was applied in the baseline scenario, while the low and high values for the sensitivity analysis were constructed by altering the baseline value ±50%. Although such variations are not always realistic, it indicates how sensitive the results are to these parameters. All parameters and values tested in the sensitivity analysis are provided in Section S1 in the SI.

CALCULATIONS

The life cycle inventory (LCI) data for DND and diamond film production are described in the following sections. A summary of the data applied in the LCI calculations is provided in Section S1 in the SI. A description of how to obtain unit-process data for the production of diamond film with a specific thickness different from the 10 μm applied in this study is provided in Section S3.1 in the SI.

Production of Nanodiamond. *Detonation Synthesis.* DNDs are formed by detonating carbon-containing explosives that release large amounts of energy.[5] The explosives are detonated in a chamber with a typical volume of 2−5 m^3 for 0.1−1 kg explosive charges,[36,37] where high-pressure and high-temperature conditions exist for a fraction of a microsecond.[5] The detonation chambers are simple in operation and have a long operating life.[37] The explosive is typically composed of 40−60% 2,4,6-trinitrotoluene (TNT), and the remainder is 1,3,5-trinitroperhydro-1,3,5-triazine (RDX).[5] In commercial production, the chamber is filled with water as coolant[6] and the yield of the resulting detonation soot is about 10% of the explosive charge.[36] During detonation of explosives, blasting gases are formed and emission factors from the US EPA[38] were applied to estimate types and amounts of gases from TNT and RDX detonation (see Table S1 in the SI). The explosion gases were assumed to be emitted to air. The resulting detonation soot contains 75% DND aggregates consisting of primary particles (4−5 nm) as well as nondiamond carbon allotropes and impurities.[4] However, the amount of DND aggregates in

https://doi.org/10.1021/acssuschemeng.3c05854
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the detonation soot can vary between 30 and 80% depending on the conditions.[5] Metallic impurities originating from, e.g., the igniter and the steel walls of the detonation chamber, constitute 1−8% and the remainder is nondiamond carbon allotropes.[5]

Purification. The detonation soot needs to be purified, which is typically performed in connection with the detonation synthesis to remove nondiamond carbon and metallic impurities.[5] First, the water coolant used in the detonation synthesis is mechanically removed by sieving and was assumed to become liquid aqueous waste. Then, the detonation soot is subjected to thermal oxidation with strong liquid oxidizers at elevated temperatures and pressures,[5] about 230 °C and 8−10 MPa.[37] Nitric acid (HNO_3) is the most commonly used oxidizer[26,39] and its initial concentration should be at least 50−60%.[26] A concentration at 60% HNO_3 is applied in industrial synthesis and the detonation soot is exposed to such HNO_3 solutions under high temperature and pressure for about 35 min.[37] A 100% yield of purified DNDs from the detonation soot was assumed since DNDs are chemically inert and hardly oxidizable, contrary to other carbons.[37] The range of 90−100% yield was tested in the sensitivity analysis since lower yields were deemed unlikely. During thermal oxidation, DND aggregates become separated as metal impurities dissolve and the nondiamond carbon oxidizes[37,40]

$$2HNO_3 + C \rightarrow CO_2 + NO_2 + NO + H_2O \tag{R1}$$

After purification, the DND powder typically consists of 80−90% carbon phase (90−99% diamond and 1−10% nondiamond[5]), 0.5−5% residues, such as metallic impurities, and the rest is oxygen, hydrogen, and nitrogen.[41]

The amount of HNO_3 was estimated based on the nondiamond carbon allotropes that becomes oxidized in the purification process, $m_{\text{non-d,ox}}$ [g], the stoichiometry of reaction R1 and a yield at 95%.[42] In turn, $m_{\text{non-d,ox}}$ was calculated based on the difference in nondiamond carbon between the detonation soot and the purified DND powder. For this, data on the detonation soot carbon phase composition (see the Detonation Synthesis section) was applied together with the yield of aggregated DNDs in the purification process, $Y_{\text{p,DND}}$ [%], and the share of DND in the purified DND powder's carbon phase, $w_{\text{p,c,DND}}$ [%]

$$m_{\text{non-d,ox}} = m_{\text{ds}} \cdot w_{\text{ds,non-d}} - \frac{m_{\text{ds}} \cdot w_{\text{ds,DND}} \cdot Y_{\text{p,DND}}}{w_{\text{p,c,DND}}} \cdot (1 - w_{\text{p,c,DND}}) \tag{1}$$

where m_{ds} is the input of detonation soot to the purification [g], $w_{\text{ds,non-d}}$ is the share of detonation soot input that is nondiamond carbon, and $w_{\text{ds,DND}}$ is the share of detonation soot input that is DND [%].

Reaction outputs from the purification (CO_2, NO_2, NO, and H_2O) were all estimated based on the stoichiometry of reaction R1. According to Dolmatov,[37] the industrial thermal oxidation treatment of detonation soot involves the recovery and utilization of acid gases as well as the recycling of nitric acid. The degree of recovery was, however, not stated, and therefore, a 50% recovery rate of acid vapors and gases (i.e., the reaction products of NO_2 and NO in reaction R1) was assumed while the range 0−100% was tested in the sensitivity analysis. Similarly, a recovery rate at 50% of unreacted HNO_3 was assumed while the range 0−100% was tested in the sensitivity analysis. The unrecovered reaction products in reaction R1 were assumed to be emitted to air. Unreacted HNO_3 that does not become recovered, together with the water from the nitric acid solution and dissolved metal impurities from the detonation soot, were assumed to become liquid aqueous waste.

Due to limited data in the literature, the energy needed for heating during thermal oxidation was calculated based on Piccinno et al.,[43] who provide an engineering-based approach to estimate industrial-scale heating in liquid batch reactions. Further details on the data applied for the electricity calculation are presented in Table S1 in the SI.

Disaggregation. After purification, the DND particles are present as aggregates with sizes ranging from a few hundred nanometers to micrometers and need to be disaggregated.[4] The conventional disaggregation techniques include wet ball milling and bead-assisted sonic disintegration, which both rely on mechanical forces assisted by zirconium dioxide (ZrO_2) microbeads.[44] According to Shenderova and Nunn,[5] wet high-energy ball milling is likely the most applied technology for disaggregation of DNDs, in which a milling media (typically ZrO_2),[44] a solvent and DND powder from the purification process are mixed in a sealed container and rotated at high speed. In such wet milling, the container's chamber is filled with milling media at 70−80 vol %.[45] The remaining 20−30 vol % is filled with a suspension containing about 10% DND aggregates, and the solvent.[46] The resulting output is primary spherical DND particles with an average size of 4−5 nm.[5]

Monodispersed DND particles with an average particle size at 5 nm are commercially sold with both DMSO and deionized water.[47] DMSO was considered in the baseline scenario and deionized water solvent was considered in the scenario analysis. The small amounts of uncrushed aggregates that remain in the disaggregation process are removed by filtration and centrifugation.[46] The process yield was not stated, but since only small amounts remain uncrushed, a yield of 95% was applied in the baseline scenario and the narrow range 90−100% was tested in the sensitivity analysis. The uncrushed DND powder was assumed to become solid waste from this process. The inputs of DND aggregates, $m_{\text{DND,dp,in}}$ [g] and solvent, $m_{\text{solvent,dp,in}}$ [g] to the disaggregation process were calculated according to

$$m_{\text{DND,dp,in}} = m_{\text{DND,dp,out}} + \frac{m_{\text{DND,dp,out}}}{Y_{\text{dp}}} \cdot (1 - Y_{\text{dp}}) \tag{2}$$

$$m_{\text{solvent,dp,in}} = \frac{m_{\text{DND,dp,in}}}{w_{\text{dp}}} \cdot (1 - w_{\text{dp}}) \tag{3}$$

where $m_{\text{DND,dp,out}}$ is the output of primary DND particles from the disaggregation process [g], Y_{dp} is the yield of primary DND particles over the disaggregation process [%], and w_{dp} is the share of aggregated DNDs in the suspension input to the disaggregation process [%]. For these calculations, $m_{\text{DND,dp,out}}$ was set equal to 1 g, i.e., the functional unit for DND production.

It was assumed that 100% of the milling media can be reused many times, so no input of ZrO_2 was considered in the baseline scenario. This assumption was tested in the sensitivity analysis by considering the case where 0% of the milling media becomes reused but instead sent to recycling after the disaggregation process. In that case, the ZrO_2 input was estimated from the weight of the suspension input ($m_{\text{DND,dp,in}}$

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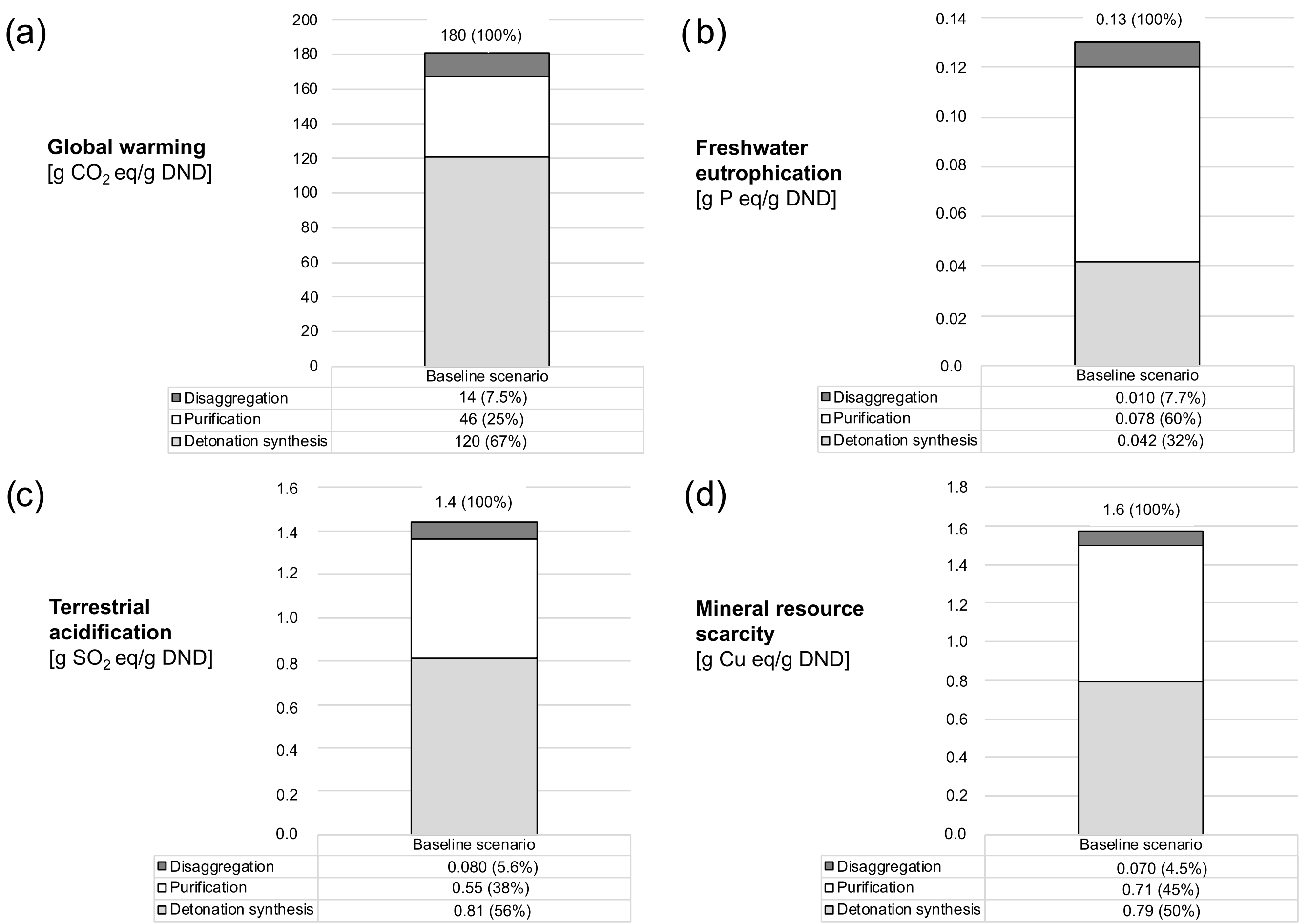

Figure 3. Life cycle impact assessment (LCIA) results for (a) global warming, (b) freshwater eutrophication, (c) terrestrial acidification, and (d) mineral resource scarcity for industrial production of detonation nanodiamond (DND) in the baseline scenario. The results are presented with two significant numbers per functional unit, i.e., 1 g nanodiamonds (4−5 nm primary particles).

and $m_{solvent,dp,in}$), the densities of purified DND powder/solvent/ZrO_2 and 75 vol % ZrO_2 milling media in the chamber (the suspension constitutes the rest).[45,46]

After disaggregation, fractionation is needed to obtain a narrower size distribution with 4−5 nm primary DND particles, which is performed through centrifugation.[5] Due to limited data, generic electricity inputs at 16 kWh/ton of ground material for disaggregation and 10 kWh/ton dry material for centrifugation were assumed based on Piccinno et al.[43]

Production of Diamond Film. Diamond film production via MWCVD utilizes gas as a precursor, consisting of methane (CH_4) and hydrogen (H_2) from which carbon is deposited onto a substrate.[3] Large-scale commercialized diamond film production is typically conducted using a 915 MHz operating frequency apparatus[48] with a power of 30−60 kW[27] accommodating a substrate of about 15 cm in diameter.[49] The diamond film growth rate is 1−12 μm/h depending on the application.[27] In the baseline scenario, a power of 45 kW and a growth rate of 6.5 μm/h were applied to calculate the electricity required to grow a 10-μm thick diamond film on the 15 cm diameter substrate.

Silicon (Si) substrates are commonly applied in polycrystalline diamond film deposition[1] and therefore considered here. When such nondiamond substrates are used, they are first seeded with fine diamond particles that serve as nucleation centers. Electrostatic seeding is currently the most widely used seeding technique in polycrystalline diamond film synthesis,[50] in which the substrate is dipped in a suspension with monodispersed DNDs. The DMSO solvent accompanying the DNDs in the suspension was assumed to become liquid organic waste in this process. More than 10^{11} DNDs per cm^2 is required for growing diamond films <50 nm, while much lower seed numbers can be applied if thicker films are grown.[50] Gracio et a.[51] reported that in the process of coating metals with diamond, more than 10^8 DNDs per cm^2 is required. The weight of nanodiamonds required for the seeding in the baseline scenario was estimated based on 10^{11} DNDs per cm^2,[50] a substrate diameter of 15 cm,[49] a spherical particle size at 4.5 nm in diameter[5] and a nanodiamond density of 3200 kg/m^3.[52]

Typical deposition conditions involve pressures and temperatures at 0.67−13 kPa and 800−1000 °C, respectively,[28] under which the following deposition takes place[53]

$$CH_4(g) \rightarrow C(diamond) + 2H_2(g) \quad (R2)$$

The weight of the grown diamond film, excluding DND seeds, was calculated based on the substrate diameter, the diamond film thickness, and the typical density of CVD-grown diamond (2800−3510 kg/m^3).[27] The stochiometric input of CH_4 to the MWCVD synthesis was then calculated based on reaction R2. The input of H_2 was calculated based on a typical

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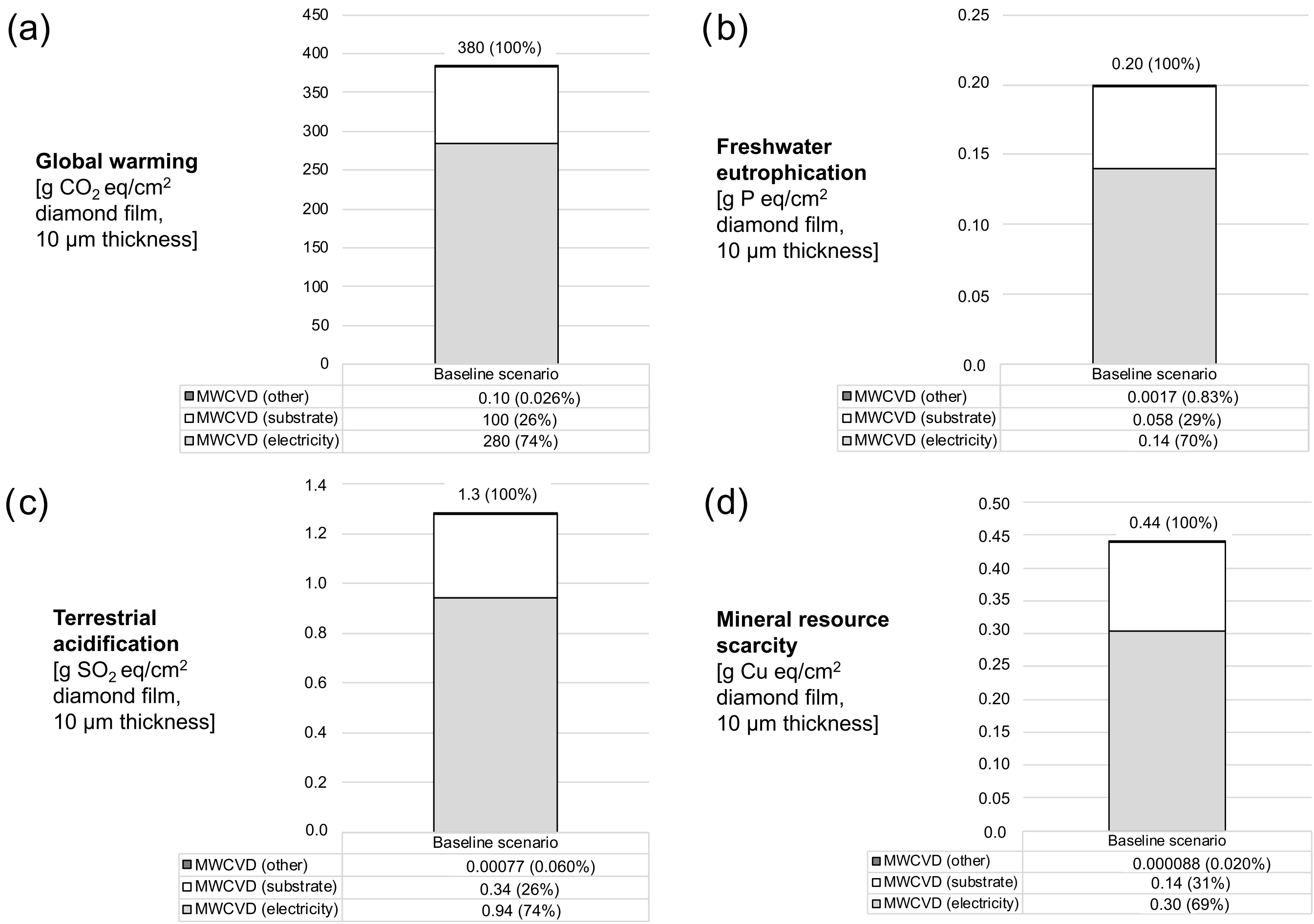

Figure 4. Life cycle impact assessment (LCIA) results for (a) global warming, (b) freshwater eutrophication, (c) terrestrial acidification, and (d) mineral resource scarcity for industrial diamond film production via microwave chemical vapor deposition (MWCVD) synthesis in the baseline scenario. The results are presented with two significant numbers per functional unit, i.e., 1 cm^2 diamond film with a 10 μm thickness.

gas composition of CH_4 and H_2 at 1 and 99 vol %, respectively.[54] It was assumed that all CH_4 input reacts into diamond in this process and that the H_2 (both from the input gas and from reaction R2) becomes vented to air via an exhaust system as indicated by Wahl et al.[55]

After the MWCVD synthesis, a diamond film with a specific thickness has been deposited on the substrate. The substrate was included in the unit-process data in this study as a part of the final product, i.e., a diamond film on a Si substrate. The thickness of the Si substrate (or wafer) was assumed at 775 μm based on a Chinese Si wafer manufacturer.[56] According to Palyanov et al.,[1] thick diamond films can be separated from the substrate to obtain a free-standing diamond wafer, but this separation was not considered in this study.

■ RESULTS AND DISCUSSION

In this section, the unit-process data and LCIA results for the four impact categories in focus are presented. LCIA results for all impact categories in the ReCiPe 2016 midpoint method are provided in Section S7 in the SI.

Nanodiamond Production Impacts. The largest inputs to DND production are water used for cooling (72 kg) and TNT plus RDX explosives (5.6 g each) in detonation synthesis as well as the input of DMSO solvent (9.5 g) in the disaggregation process. The largest energy input is the 0.0013 kWh electricity used in the disaggregation process. The unit-process data results for DND production are shown in Table S3 in the SI.

The LCIA results for global warming, freshwater eutrophication, terrestrial acidification and mineral resource scarcity are shown in Figure 3. The figure shows that detonation synthesis is the main contributor to global warming, terrestrial acidification, and mineral resource scarcity, while purification dominates freshwater eutrophication. For global warming, the inputs of TNT/RDX explosives and large amounts of tap water used for cooling (mainly the electricity used in tap water production) in detonation synthesis constitute hotspots at about 35 and 31%, respectively. The subsequent treatment of the large amounts of wastewater from the purification process also contributes notably at about 22%. This is mainly related to the construction of sewer grids, construction of wastewater treatment facility, and the use of electricity in the treatment process. The main contributors to freshwater eutrophication are the treatment of wastewater from the purification process (about 63%), mainly due to emissions of nutrients from this process, and the input of tap water to detonation synthesis (about 25%). The contribution from the input of tap water is largely due to electricity use in tap water production from, e.g., lignite sources and the associated landfill treatment of spoil materials from mining operations. Emissions of blasting gases from detonation synthesis and the inputs of TNT/RDX explosives and tap water to this process contribute at about 28,

https://doi.org/10.1021/acssuschemeng.3c05854
ACS Sustainable Chem. Eng. 2024, 12, 365−374

15, and 13%, respectively, to terrestrial acidification. In addition, the treatment of wastewater from the purification process contributes at 19% due to, e.g., hard coal mining operations related to the use of electricity in wastewater treatment. Regarding mineral resource scarcity, the treatment of wastewater in the purification process, largely related to the use of clay and steel in treatment facility and sewer grid construction, is responsible for 45% of the impact. The tap water input to the detonation synthesis contributes at about 39% of the total impact, mainly due to the use of cast iron in water supply network construction and aluminum sulfate powder in tap water production.

The global warming impacts of DND and synthetic diamond grit can be compared because they have similar properties and are used in similar applications, such as polishing.[4,48] Specifically, the impact of 1 g DND (baseline scenario in this study) was compared to 1 g synthetic diamond grit (HPHT production according to the "current scenario" in Furberg et al.[11]). The comparison shows that the global warming impact of synthetic diamond grit (about 920 g CO_2 equiv/g) is about 5 times higher than the impact of DND (about 180 g CO_2 equiv/g). Thus, in applications where these materials provide similar function(s), DND is preferable from a global warming perspective.

Diamond Film Production Impacts. The largest material input to the diamond film production via MWCVD is the 0.18 g Si substrate and about 0.38 kWh electricity is required. The unit-process data results for diamond film via MWCVD are provided in Table S7 in the SI.

The LCIA results for global warming, freshwater eutrophication, terrestrial acidification, and mineral resource scarcity for the baseline scenario are shown in Figure 4. The electricity and substrate inputs clearly dominate all of the environmental impacts at 69−74 and 26−31%, respectively. Considerable amounts of electricity are required in the diamond film production and in the baseline scenario, this is modeled as global average electricity, which is largely fossil-based. For the Si substrate production, it is also the upstream electricity requirement that mainly contributes to global warming. For freshwater eutrophication, it is the landfill treatment of spoil materials from, e.g., lignite and hard coal mining related to electricity generation, that contributes the most. In addition, hard coal mining for electricity generation contributes notably to terrestrial acidification. For mineral resource scarcity, the use of resources related to electricity generation (e.g., steel in the construction of hard coal mines) and various resources in Si substrate production (e.g., hydrochloric acid) contribute the most.

Opportunities for Reducing Impacts. In this section, potentials for reducing the environmental and resource impacts of DND and diamond film are investigated via scenario analysis (see the Uncertainty and Sensitivity Analysis section). A shift to wind or solar power supply instead of global average electricity does not reduce impacts considerably relative to the baseline scenario for DND production. This is because the use of electricity is relatively minor (about 0.0013 kWh/g DND). In the deionized water solvent scenario, modest reductions at about 4−8% relative to the baseline scenario are achieved for the global warming, freshwater eutrophication, terrestrial acidification, and mineral resource scarcity impacts (Figure S1 in the SI). Still, changing the solvent from DMSO to deionized water is preferable from an environmental and resource perspective. There are further scenarios that could be relevant to test. For example, additional scenarios regarding the type of milling media used are relevant if the milling media is discarded after a limited number of uses. For example, milling media such as tungsten carbide and stainless steels[5] could then be tested and compared to ZrO_2. Furthermore, different solvents can be applied in wet high-energy ball milling of DNDs, including water, DMSO, methanol, and mixtures thereof,[57] which could be tested in additional scenarios. Finally, while detonation in wet synthesis takes place in the coolant water (or ice), an alternative synthesis route is dry synthesis, where the detonation takes place in a gas, such as nitrogen (N_2) or carbon dioxide (CO_2), which acts as a coolant.[5] The dry synthesis route might be interesting to compare to the wet synthesis in further studies.

Global warming, freshwater eutrophication, and terrestrial acidification impacts of diamond film production are significantly reduced relative to the baseline scenario when wind power (about 64−71% reduction) or solar power (about 62−67% reduction) is applied instead of global average electricity (Figure S2 in the SI). The mineral resource scarcity impact, however, increases with about 57 and 73% in the wind and solar power scenario, respectively. The reason for this is that wind power requires resources such as copper and steel for the construction of wind turbines and their networks. Similarly, solar power requires, e.g., copper in the production and installation of solar cells. The use of these resources in turn contributes to mineral resource scarcity. It should be noted that the mineral resource scarcity method in ReCiPe 2016 is a future-efforts method that considers the additional ore needed to extract mineral resources in the future.[58] Thus, it does not consider other resource implications, such as depletion and supply risk. Future studies might apply other methods to consider such implications, for example, the abiotic resource depletion[59] or crustal scarcity indicator[60] for depletion, and GeoPolRisk[61] or ESSENZ[62] for supply risk.

Since the substrate contributes considerably to the impact results (Figure 4), it could be interesting to investigate substrates with lower impacts in future studies. In addition to nondiamond substances such as Si, diamond itself constitutes a possible substrate.[28] In this context, the requirement for high-quality substrates and their influence on the quality of the final product should be considered. Furthermore, in addition to the 915 MHz apparatus, the 2.45 GHz apparatus is also used for diamond film production and could be tested in an additional scenario.[27] However, this reactor, applying a comparatively lower power at 6−10 kW,[27] can only accommodate smaller substrates (up to 7.5 cm in diameter).[63] Therefore, the 915 MHz reactor, which can accommodate substrates up to 20 cm,[63] was selected for this study.

Sensitivity Analysis Results. This section presents parameters causing changes in the results for the four impact categories in focus that are larger than ±10% relative to the baseline scenario, see also Section S8 in the SI. In total, eight sensitive parameters were identified to cause such changes in DND production. For four of these parameters (explosive charge per detonation (TNT/RDX), chamber volume, the NH_3 emission factor for detonation of RDX, and the composition of the detonation soot), value ranges were provided in the literature. For the other sensitive parameters (detonation soot yield, yield of aggregates in the purification process, recovery of nitrous vapors and gases, and the share of milling media reused in the disaggregation process), only single values were provided in the literature. Therefore, considering their sensitivity, efforts to obtain more realistic ranges for the latter four are recommended.

Three parameters in diamond film production caused changes larger than ±10% relative to the baseline scenario for the four impact categories in focus. These parameters (MWCVD apparatus power, growth rate, and substrate diameter) considerably affect the results for all impact categories assessed because they influence the electricity input. The power of the apparatus directly influences the electricity needed while the growth rate affects the electricity input via the number of hours required to obtain a diamond film of a specific thickness. For example, changing the growth rate from 6.5 to 1 μm/h means that about 10 h instead of 1.5 h is needed to obtain 10 μm diamond film. The substrate diameter also influences the electricity input indirectly as the diamond film area obtained is dependent on the diameter. Since a lower-range value was not provided in the literature for the substrate diameter, this parameter should be subject to further efforts to acquire a more realistic range.

CONCLUSIONS

Unit-process data and LCIA results for the global production of synthetic DND and diamond film via MWCVD are provided in response to the lack of life cycle data in the literature. The data provided in this study can be used in future cradle-to-grave LCA studies of diamond material applications. Furthermore, the unit-process data results are presented in such a way that foreground system parameters can be easily changed or updated with more specific data if such becomes available. The background system data, representing global production, can be varied in future studies to reflect production at specific locations. This was done so that the data can be adapted to the specific contexts of future studies.

The results show that a limited number of inputs dominate environmental and resource impacts: explosives and cooling water production for DND, as well as electricity and substrate production for diamond film. These hotspots are recommended to be considered by manufacturers of synthetic diamond materials to reduce impacts. The scenario analysis shows that manufacturers could consider the substitution of DMSO solvent with deionized water in DND production to reduce environmental and resource impacts. In MWCVD synthesis, changing electricity from global average to wind or solar power reduces environmental impacts considerably.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acssuschemeng.3c05854.

Section S1: Data for life cycle inventory (LCI) calculations and sensitivity analysis (including Tables S1 and S2); Section S2: Unit-process data results for nanodiamond production (including Section S2.1 Unit-process data results for nanodiamond-specific processes and Tables S3–S6); Section S3: Unit-process data results for diamond film production (including Section S3.1 Unit-process data for diamond film of a specific thickness, Tables S7 and S8 and eqs S1–S6); Section S4: Scenarios applied (including Table S9); Section S5: Description of impact categories in focus (including Table S10); Section S6: Background system data (including Tables S11 and S12); Section S7: Life cycle impact assessment (LCIA) results (including Section S7.1 Nanodiamond production, Section S7.2 Diamond film production, Figures S1 and S2 and Tables S13–S19); Section S8: Sensitivity analysis results (including Tables S20 and S21); and Section S9: References (PDF)

AUTHOR INFORMATION

Corresponding Author

Anna Furberg – *KTH Digital Futures, KTH Climate Action Center, Department of Sustainable Development, Environmental Science and Engineering, KTH Royal Institute of Technology, 100 44 Stockholm, Sweden; Norwegian Institute for Sustainability Research NORSUS, 1671 Kråkerøy, Norway;* orcid.org/0000-0001-9873-0949; Email: annafur@kth.se

Author

Rickard Arvidsson – *Division of Environmental Systems Analysis, Chalmers University of Technology, 412 96 Gothenburg, Sweden;* orcid.org/0000-0002-9258-0641

Complete contact information is available at: https://pubs.acs.org/10.1021/acssuschemeng.3c05854

Author Contributions

A.F.: Conceptualization, methodology, investigation, formal analysis, visualization, data curation, project administration, validation, writing—original draft, writing—review and editing. R.A.: Conceptualization, methodology, visualization, funding acquisition, validation, writing—review and editing.

Notes

The authors declare no competing financial interest.

ACKNOWLEDGMENTS

The financial support from Mistra Environmental Nanosafety Phase II, funded by the Swedish Foundation for Strategic Environmental Research (Mistra), is gratefully acknowledged. A.F. also acknowledges the financial support from Ericsson, KTH Digital Futures and KTH Climate Action Center.

REFERENCES

(1) Palyanov, Y. N.; Kupriyanov, I. N.; Khokhryakov, A. F.; Ralchenko, V. G. Crystal Growth of Diamond. In *Handbook of Crystal Growth*, 2nd ed.; Rudolph, P., Ed.; Elsevier, 2015; pp 671–713.

(2) USGS. (United States Geological Survey) Industrial diamond. U.S. Geological Survey, Mineral Commodity Summaries, 2023. https://www.usgs.gov/centers/national-minerals-information-center/industrial-diamond-statistics-and-information (accessed June 14, 2023).

(3) Kasu, M. Diamond epitaxy: Basics and applications. *Prog. Cryst. Growth Charact. Mater.* **2016**, *62* (2), 317–328.

(4) Kumar, S.; Nehra, M.; Kedia, D.; Dilbaghi, N.; Tankeshwar, K.; Kim, K. H. Nanodiamonds: Emerging face of future nanotechnology. *Carbon* **2019**, *143*, 678–699.

(5) Shenderova, O.; Nunn, N. Production and Purification of Nanodiamonds. In *Nanodiamonds - Advanced Material Analysis, Properties and Applications*, Arnault, J.-C., Ed.; Elsevier: 2017; pp 25–56.

(6) Vul', A. Y.; Dideikin, A. T.; Aleksenskii, A. E.; Baidakova, M. V. Detonation Nanodiamonds: Synthesis, Properties and Applications. In *Nanodiamond*; Williams, O., Ed.; RSC Nanoscience & Nanotechnology No. 31; The Royal Society of Chemistry, 2014; pp 27–48.

(7) Schwander, M.; Partes, K. A review of diamond synthesis by CVD processes. *Diamond Relat. Mater.* **2011**, *20* (9), 1287–1301.

(8) Arnault, J.-C.; Saada, S.; Ralchenko, V. Chemical Vapor Deposition Single-Crystal Diamond: A Review. *Phys. Status Solidi RRL* **2022**, *16* (1), 2100354−2100370.
(9) Keller, A. A.; Ehrens, A.; Zheng, Y.; Nowack, B. Developing trends in nanomaterials and their environmental implications. *Nat. Nanotechnol.* **2023**, *18*, 834−837.
(10) Hellweg, S.; Milà i Canals, L. Emerging approaches, challenges and opportunities in life cycle assessment. *Science* **2014**, *344* (6188), 1109−1113.
(11) Furberg, A.; Fransson, K.; Zackrisson, M.; Larsson, M.; Arvidsson, R. Environmental and resource aspects of substituting cemented carbide with polycrystalline diamond: The case of machining tools. *J. Cleaner Prod.* **2020**, *277*, 123577−123586.
(12) Ferreira, V.; Egizabal, P.; Popov, V.; García de Cortázar, M.; Irazustabarrena, A.; López-Sabirón, A. M.; Ferreira, G. Lightweight automotive components based on nanodiamond-reinforced aluminium alloy: A technical and environmental evaluation. *Diamond Relat. Mater.* **2019**, *92*, 174−186.
(13) Wilfong, C.; Gomez, H.; Durham, D. In *Life Cycle Analysis of Diamond Coating of Machining Tools*, ASME 2012 International Manufacturing Science and Engineering Conference Collocated with the 40th North American Manufacturing Research Conference and in Participation with the International Conference, MSEC, 2012; pp 1049−1056.
(14) Sun, Y.; Bai, S.; Wang, X.; Ren, N.; You, S. Prospective Life Cycle Assessment for the Electrochemical Oxidation Wastewater Treatment Process: From Laboratory to Industrial Scale. *Environ. Sci. Technol.* **2023**, *57* (3), 1456−1466.
(15) Surra, E.; Correia, M.; Figueiredo, S.; Silva, J. G.; Vieira, J.; Jorge, S.; Pazos, M.; Sanromán, M. Á.; Lapa, N.; Delerue-matos, C. Life cycle and economic analyses of the removal of pesticides and pharmaceuticals from municipal wastewater by anodic oxidation. *Sustainability* **2021**, *13* (7), 3669−3692.
(16) Arvidsson, R.; Kushnir, D.; Sandén, B. A.; Molander, S. Prospective life cycle assessment of graphene production by ultrasonication and chemical reduction. *Environ. Sci. Technol.* **2014**, *48* (8), 4529−4536.
(17) Arvidsson, R.; Nguyen, D.; Svanström, M. Life cycle assessment of cellulose nanofibrils production by mechanical treatment and two different pretreatment processes. *Environ. Sci. Technol.* **2015**, *49* (11), 6881−6890.
(18) Cossutta, M.; McKechnie, J.; Pickering, S. J. A comparative LCA of different graphene production routes. *Green Chem.* **2017**, *19* (24), 5874−5884.
(19) Li, Q.; McGinnis, S.; Sydnor, C.; Wong, A.; Renneckar, S. Nanocellulose life cycle assessment. *ACS Sustainable Chem. Eng.* **2013**, *1* (8), 919−928.
(20) Piccinno, F.; Hischier, R.; Seeger, S.; Som, C. Life cycle assessment of a new technology to extract, functionalize and orient cellulose nanofibers from food waste. *ACS Sustainable Chem. Eng.* **2015**, *3* (6), 1047−1055.
(21) Varnin, V. P.; Laptev, V. A.; Ralchenko, V. G. The state of the art in the growth of diamond crystals and films. *Inorg. Mater.* **2006**, *42* (Suppl. 1), S1−S18.
(22) Finnveden, G.; Hauschild, M. Z.; Ekvall, T.; Guinée, J.; Heijungs, R.; Hellweg, S.; Koehler, A.; Pennington, D.; Suh, S. Recent developments in Life Cycle Assessment. *J. Environ. Manage.* **2009**, *91* (1), 1−21.
(23) Baumann, H.; Tillman, A.-M. *The Hitchhiker's Guide to LCA: An Orientation in Life Cycle Assessment Methodology and Application*, Studentlitteratur: 2004; pp 1−543.
(24) Sauer, B. Life Cycle Inventory Modelling in Practice. In *Life Cycle Assessment Handbook: A Guide for Environmentally Sustainable Products*, 1st ed.; Curran, M. A., Ed.; John Wiley & Sons, Incorporated, 2012; pp 43−66.
(25) Furberg, A.; Arvidsson, R.; Molander, S. A practice-based framework for defining functional units in comparative life cycle assessments of materials. *J. Ind. Ecol.* **2022**, *26* (3), 718−730.
(26) Osswald, S. Nanodiamond Purification. In *Nanodiamond*, Williams, O., Ed.; RSC Nanoscience & Nanotechnology No.31, The Royal Society of Chemistry, 2014; pp 89−111.
(27) Gupta, T. The Transparent Carbon: the Diamond. In *Carbon. The Black, the Gray and the Transparent*, Gupta, T., Ed.; Springer International Publishing, 2018; pp 259−298.
(28) Kreuger, A. Diamond Films. In *Carbon Materials and Nanotechnology*; Wiley-VCH, 2010; pp 389−449.
(29) Gavankar, S.; Suh, S.; Keller, A. A. The Role of Scale and Technology Maturity in Life Cycle Assessment of Emerging Technologies: A Case Study on Carbon Nanotubes. *J. Ind. Ecol.* **2015**, *19* (1), 51−60.
(30) Ekvall, T.; Björklund, A.; Sandin, G.; Jelse, K.; Lagergren, J.; Rydberg, M. *Modeling Recycling in Life Cycle Assessment. Report Number: 2020:05*; Swedish Life Cycle Center: Gothenburg, Sweden, 2020. https://www.lifecyclecenter.se/publications/modeling-of-recycling-in-life-cycle-assessment/ (accessed June 30, 2022).
(31) Huijbregts, M. A. J.; Steinmann, Z. J. N.; Elshout, P. M. F.; Stam, G.; Verones, F.; Vieira, M.; Zijp, M.; Hollander, A.; van Zelm, R. ReCiPe2016: a harmonised life cycle impact assessment method at midpoint and endpoint level. *Int. J. Life Cycle Assess.* **2017**, *22* (2), 138−147.
(32) Ecoinvent Database v3.7, 2020. https://ecoinvent.org (accessed July 30, 2023).
(33) Häggvall, J.; Hochschomer, E.; Finnveden, G.; Overcash, M.; Griffing, E. *Life Cycle Assessment of a PFHE Shell Grenade. Report number: FOI-R—1373—SE*; Swedish Defence Research Agency. November 2004; 2004. https://www.foi.se/rapportsammanfattning?reportNo=FOI-R--1373--SE (accessed December 22, 2022).
(34) Ferreira, C. M. B. Extended Environmental Life-Cycle Assessment of Munitions: Addressing Chemical Toxicity Hazard on Human Health. Ph.D. Thesis, University of Coimbra, 2017.
(35) Igos, E.; Benetto, E.; Meyer, R.; Baustert, P.; Othoniel, B. How to treat uncertainties in life cycle assessment studies? *Int. J. Life Cycle Assess.* **2019**, *24* (4), 794−807.
(36) Danilenko, V.; Shenderova, O. A. Advances in Synthesis of Nanodiamond Particles. In *Ultrananocrystalline Diamond - Synthesis, Properties and Applications*, 2nd ed.; Shenderova, O. A.; Gruen, D. M., Eds.; Elsevier, 2012; pp 133−164.
(37) Dolmatov, V. Y. Detonation-synthesis nanodiamonds: synthesis, structure, properties and applications. *Russ. Chem. Rev.* **2007**, *76* (4), 339−360.
(38) US EPA. (United States Environmental Protection Agency) Detonation of Explosives: An AP-42 Update. EPA-450/4−79−023, 1979. https://nepis.epa.gov/Exe/ZyNET.exe/9100A0MG.TXT?ZyActionD=ZyDocument&Client=EPA&Index=1976+Thru+1980&Docs=&Query=&Time=&EndTime=&SearchMethod=1&TocRestrict=n&Toc=&TocEntry=&QField=&QFieldYear=&QFieldMonth=&QFieldDay=&IntQFieldOp=0&ExtQFieldOp=0&XmlQuery=&File=D%3A%5Czyfiles%5CIndex%20Data%5C76thru80%5CTxt%5C00000012%5C9100A0MG.txt&User=ANONYMOUS&Password=anonymous&SortMethod=h%7C-&MaximumDocuments=1&FuzzyDegree=0&ImageQuality=r75g8/r75g8/x150y150g16/i425&Display=hpfr&DefSeekPage=x&SearchBack=ZyActionL&Back=ZyActionS&BackDesc=Results%20page&MaximumPages=1&ZyEntry=1&SeekPage=x&ZyPURL (accessed Dec 23, 2022).
(39) Shugalei, I. V.; Ilyushin, M. A.; Sudarikov, A. M. Preparation of complex nitric fertilizers during recycling of acidic wastes of detonation nanodiamonds purification stage. *Russ. J. Gen. Chem.* **2014**, *84* (13), 2539−2541.
(40) Sushchev, V. G.; Dolmatov, V. Y.; Marchukov, V. A.; Veretennikova, M. V. Fundamentals of chemical purification of detonation nanodiamond soot using nitric acid. *J. Superhard Mater.* **2008**, *30* (5), 297−304.
(41) Kreuger, A. Nanodiamond. In *Carbon Materials and Nanotechnology*, Wiley-VCH: 2010; pp 329−388.

(42) Hischier, R.; Hellweg, S.; Capello, C.; Primas, A. Establishing Life Cycle Inventories of Chemicals Based on Differing Data Availability. *Int. J. Life Cycle Assess.* **2005**, *10* (1), 59−67.
(43) Piccinno, F.; Hischier, R.; Seeger, S.; Som, C. From laboratory to industrial scale: a scale-up framework for chemical processes in life cycle assessment studies. *J. Cleaner Prod.* **2016**, *135*, 1085−1097.
(44) Terada, D.; So, F. T.; Hattendorf, B.; Yanagi, T.; Osawa, E.; Mizuochi, N.; Shirakawa, M.; Igarashi, R.; Segawa, T. F. A simple and soft chemical deaggregation method producing single-digit detonation nanodiamonds. *Nanoscale Adv.* **2022**, *4*, 2268−2277.
(45) Osawa, E.; Sasaki, S.; Yamanoi, R. Deagglomeration of Detonation Nanodiamond. In *Ultrananocrystalline Diamond - Synthesis, Properties and Applications*, 2nd ed.; Shenderova, O. A.; Gruen, D. M., Eds.; Elsevier, 2012; pp 165−179.
(46) Ōsawa, E. Monodisperse single nanodiamond particulates. *Pure Appl. Chem.* **2008**, *80* (7), 1365−1379.
(47) Sigma-Aldrich. Monodispersed Nanodiamond Particles, 2022. https://www.sigmaaldrich.com/SE/en/product/aldrich/900180 (accessed Dec 29, 2022).
(48) Vohler, O.; Nutsch, G.; Von Sturm, F.; Wege, E. Carbon, 2. Diamond. In *Ullmann's Encyclopedia of Industrial Chemistry*; Wiley-VHC Verlag GmbH & Co. KGaA, 2010.
(49) Kobashi, K. Microwave Plasma CVD Reactors. In *Diamond Films. Chemical Vapor Deposition for Oriented and Heteroepitaxial Growth*; Elsevier, 2005; pp 17−22.
(50) Mandal, S. Nucleation of diamond films on heterogeneous substrates: a review. *RSC Adv.* **2021**, *11* (17), 10159−10182.
(51) Gracio, J. J.; Fan, Q. H.; Madaleno, J. C. Diamond growth by chemical vapour deposition. *J. Phys. D: Appl. Phys.* **2010**, *43* (37), 374017−374038.
(52) American Elements. Diamond Nanoparticles, 2023. https://www.americanelements.com/diamond-nanoparticles-7782-40-3 (accessed Jan 09, 2023).
(53) Pierson, H. O. CVD Diamond. In *Handbook of Carbon, Graphite, Diamonds and Fullerenes*; Pierson, H. O., Ed.; William Andrew Publishing, 1993; pp 302−336.
(54) Gomez Vega, H. A. Interface Engineered Diamond Coatings for Dry Machining Applications. Ph.D. Thesis, University of South Florida, 2011.
(55) Wahl, G.; Davies, P. B.; Bunshah, R. F.; Joyce, B. A.; Bain, C. D.; Wegner, G.; Remmers, M.; Walsh, F. C.; Hieber, K.; Sundgren, J.-E.; Bachman, P. K.; Miyazawa, S.; Thelen, A.; Strathmann, H.; Edler, K. J. Thin Films. In *Ullmann's Encyclopedia of Industrial Chemistry*; Wiley-VCH Verlag GmbH & Co. KGaA, 2014.
(56) PAM-XIAMEN. 12" Prime Grade Silicon Wafer, 2023. https://www.powerwaywafer.com/silicon-wafer/300mm-bare-silicon-wafers-prime-grade.html (accessed Jan 07, 2023).
(57) Krueger, A.; Ozawa, M.; Jarre, G.; Liang, Y.; Stegk, J.; Lu, L. Deagglomeration and functionalisation of detonation diamond. *Phys. Status Solidi A* **2007**, *204* (9), 2881−2887.
(58) Sonderegger, T.; Berger, M.; Alvarenga, R.; Bach, V.; Cimprich, A.; Dewulf, J.; Frischknecht, R.; Guinée, J.; Helbig, C.; Huppertz, T.; Jolliet, O.; Motoshita, M.; Northey, S.; Rugani, B.; Schrijvers, D.; Schulze, R.; Sonnemann, G.; Valero, A.; Weidema, B. P.; Young, S. B. Mineral resources in life cycle impact assessment—part I: a critical review of existing methods. *Int. J. Life Cycle Assess.* **2020**, *25* (4), 784−797.
(59) van Oers, L.; Guinée, J. B.; Heijungs, R. Abiotic resource depletion potentials (ADPs) for elements revisited—updating ultimate reserve estimates and introducing time series for production data. *Int. J. Life Cycle Assess.* **2020**, *25* (2), 294−308.
(60) Arvidsson, R.; Söderman, M. L.; Sandén, B. A.; Nordelöf, A.; André, H.; Tillman, A. M. A crustal scarcity indicator for long-term global elemental resource assessment in LCA. *Int. J. Life Cycle Assess.* **2020**, *25* (9), 1805−1817.
(61) Gemechu, E. D.; Sonnemann, G.; Young, S. B. Geopolitical-related supply risk assessment as a complement to environmental impact assessment: the case of electric vehicles. *Int. J. Life Cycle Assess.* **2017**, *22* (1), 31−39.
(62) Bach, V.; Berger, M.; Henßler, M.; Kirchner, M.; Leiser, S.; Mohr, L.; Rother, E.; Ruhland, K.; Schneider, L.; Tikana, L.; Volkhausen, W.; Walachowicz, F.; Finkbeiner, M. Integrated method to assess resource efficiency − ESSENZ. *J. Cleaner Prod.* **2016**, *137*, 118−130.
(63) Rats, D.; Provent, C. CVD Reactor for Manufacturing Synthetic Films and Methods of Fabrication. World Intellectual Property Organisation (WIPO) International Bureau. WO2021/069620 A1, 2021.