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DESIGN FOR ADDITIVE MANUFACTURING – UTILIZATION STUDY FOR A NOVEL APPLICATION AREA

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TIIVISTELMÄ

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Suunnittelu lisäävälle valmistukselle – hyödyntämistutkimus uudelle käyttöalueelle

Diplomityö

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70 sivua, 32 kuvaa, 2 taulukkoa

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Lisäävän valmistustekniikan täysimääräinen hyödyntäminen edellyttää valmistusprosessien tuntemista, jota DfAM (Design for Additive Manufacturing) suunnitteluperiaate tukee hyvin. DfAM käsittää suunnittelumenetelmät ja teknologiat, mitä lisäävä valmistustekniikka pystyy hyödyntämään sekä parhaat tuotesuunnittelun käytännöt valmistustekniikan rajoitteiden huomioimiseksi. DfAM -metodiikka ei kuitenkaan ole vain kokoelma erinäisiä suunnitteluohjeita, vaan kattaa koko valmistusprosessin minimoiden tekniset ja taloudelliset riskit.

Tämä diplomityö tutkii DfAM-suunnitteluperiaatteen soveltamista energeettisten materiaalien (EM) lisäävän valmistuksen tuotesuunnitteluun. Kirjallisuusosiossa selvitettiin yleisesti tunnistetut DfAM-metodit sekä esiteltiin prosessikuvaus. Tätä tarkasteltiin energeettisten materiaalien ominaisuuksiin ja toimintaperiaatteisiin tavoitteena sovittaa yhteen ja saavuttaa ymmärrys lisäävän valmistustekniikan mahdollisuuksista uuden käyttöalueen kanssa.

Energeettisiä materiaaleja ei välttämättä pystytä optimoimaan lisäävälle valmistustekniikalle, eivätkä kaupalliset tulostinsovellukset ole suoraan EM materiaaleille soveltuvia. Kirjallisuusosiossa esiteltiin ideaalisen tulostusmateriaalin reologia Material extrusion (MEX) pursotus tekniikalle.

Kokeellisessa osassa suunniteltiin perinteisille EM valmistustekniikoille mahdoton prototyyppikappale soveltamalla kirjallisuusosuudessa tutkittuja DfAM-suunnitteluperiaatteita. Jatkotutkimuksia vaaditaan kappaleen turvallisen tulostamisen ja suorituskyvyn validoimiseksi. Vahvimpina mahdollisuuksina nähdään topologia optimoinnin kehittäminen ja EM materiaalien huokoisuuden hyödyntäminen painevaikutuksen optimoimiseksi.

ABSTRACT

LUT University
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Design for additive manufacturing – utilization study for a novel application area

Master's thesis

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70 pages, 32 figures, 2 table

Examiners: Professor, Heidi Piili, D.Sc. (Tech.)
Postdoctoral researcher, Amir Toghyani, D.Sc. (Tech.)

Keywords: AM, additive manufacturing, design, 3D-printing, energetic materials, DfAM

The full utilization of additive manufacturing requires understanding of manufacturing processes, which the design for additive manufacturing (DfAM) methodology supports well. The DfAM methodology comprises of design methods and technologies that additive manufacturing can utilize, and the best design practices adapted to take account of manufacturing constraints. However, the DfAM methodology is not just a collection of different design guidelines, instead it covers the whole additive manufacturing value chain to minimize technical and economic risks.

This thesis researches the utilization of the DfAM methodology on the design of energetic materials' (EM) additive manufacturing. On the literature review section, common DfAM design methods were visited and the DfAM process was introduced. This was investigated against the properties and operating principles of energetic materials (EM), with the objective of recognizing and gaining understanding of the value adding opportunities of additive manufacturing for the novel application area.

Energetic materials may not be able to be optimized for additive manufacturing technology, and commercial printer applications are not directly suitable for energetic materials. On the literature review section, the rheology of an ideal printing material for the material extrusion (MEX) technique was introduced.

In the experimental section, a prototype part impossible for traditional EM manufacturing methods was designed by applying the DfAM design principles reviewed in the literature section. Further research is required to validate the safe printing and performance of the part. The development of topology optimization and the utilization of energetic materials' porosity for the optimization of the pressure effect was seen as the most promising opportunity.

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LIST OF SYMBOLS AND ABBREVIATIONS

α	Overhang angle
$\dot{\gamma}$	Shear rate
η	Viscosity
ρ	Density
σ	Stress
σ_y^{dyn}	yield stress
τ	Shear stress
τ_y	Yield stress
h	Height
g	Gravity constant
G′	Elastic moduli
G″	Viscous moduli
S	Printing speed
$\dot{Q}$	Volumetric flow rate
AM	Additive manufacturing
ASTM	American society for testing and materials
BJT	Binder jetting
CAD	Computer aided engineering
CEN	European committee
CFD	Computational fluid dynamics
DED	Directed energy deposition
FDM	Fused deposition modeling
DfAM	Design for additive manufacturing
DfMA	Design for manufacturing and assembly
DIW	Direct ink writing
EM	Energetic material
EN	European Standards
EOS	Equation of state

FE	Finite element
FEA	Finite element analysis
FEM	Finite element method
GD	Generative design
HE	High-Explosive
ISO	International Organization for Standardization
LE	Low explosive
MEX	Material extrusion
MJT	Material jetting
PBF	Powder bed fusion
SHL	Sheet lamination
SIMP	Solid isotropic microstructure with penalisation
SLS	Selective laser sintering
STL	STereoLithography
TO	Topology optimization
TPMS	Triply periodic minimal surface
ZND	Zeldovich-Neumann-Doering
VPP	Vat photopolymerization

1 INTRODUCTION

Additive manufacturing (AM) is defined as a manufacturing method to produce items by combining materials together, typically layer by layer and so that at the same time, both the basic geometry and the desired basic material properties are achieved (EN ISO/ASTM 52900). Additive manufacturing allows for the creation of objects without geometrical limitations, and more importantly parts can be designed with functional requirements in priority. Additive manufacturing is contrary to traditional manufacturing methods that often require machining or other techniques to shape material. (Diegel et al. 2019, p. 2) Due to this essential difference, new aspects need to be embedded into the product design methodology as well.

Cost sub-respondent status, quality of the parts, manufacturability and other aspects can be improved by designing the parts specifically to suit additive manufacturing technology. Design for additive manufacturing (DfAM) is a collection of different methods that can be applied to take full advantages of the AM technologies. The products must be specifically designed for additive manufacturing, otherwise they are not even worth doing with AM (Diegel et al. 2019, p. 132). The lack of knowledge on DfAM has been identified as one of the barriers that holds back further adoption of additive manufacturing (Vaneker et al. 2020, p. 579).

1.1 Background

Energetic materials (EM) are substances that store large amounts of chemical energy which can be released rapidly. The effect of aspect ratio, shape, and location of an initiation point could be as effective and profitable to the performance of energetic materials as the chemical composition or mass of the product itself. (Knock C. & Davies N. 2013 p.337)

Traditional EM manufacturing methods, such as casting, pressing and extrusion, represent the formative manufacturing approach and are therefore relatively limited methods when it comes to the shape complexity. Demand for size and cost reduction while increasing safety and maintaining the performance of energetic products remains a challenge for traditional tools and technologies (Muravyev N. et al. 2019 p.941). However, fabrication of complex shapes is not a problem for additive manufacturing processes.

1.2 Aim, framing and methods of the research

The research method consists of literature review and experimental part. The main motivation for this thesis was to reconcile the potential of additive manufacturing with a novel energetic material application area. This was done by utilizing DfAM methodology to recognize the EM product characteristics to which additive manufacturing capabilities reflect and could add value. The EM characteristics and the DfAM methods are visited in the literature review part.

Due to unstable nature, composition and additional safety requirements, standard additive manufacturing processes do not directly apply to the fabrication of energetic materials. Material rheology is a core element in successful additive manufacturing processes. The rheology and printability of an ideal material are reviewed in the literature part.

The experimental part focuses on the design of an EM product unobtainable with traditional manufacturing technologies to demonstrate the DfAM methodology. Design guidelines for manufacturability are investigated, and a simple prototype design for additive manufacturing is proposed. The hypothesis is that by utilizing DfAM, value adding opportunities can be identified and the methodology will help engineers to design parts optimized for additive manufacturing.

2 LITERATURE REVIEW

2.1 Additive manufacturing

Additive manufacturing is globally a more and more industrially used method whereby a part is manufactured based on the 3D geometry description with substance addition techniques. Standardization has a crucial role in building confidence in additive manufacturing as an industrial production technology. Standardization ensures that the products and systems are compatible and able to work together.

The international standardization organization concerning additive manufacturing is ISO/TC 261 on additive manufacturing technical committee. The corresponding European committee is CEN/TC 438 - Additive Manufacturing. Currently ISO/TC 261 has published 19 standards and 28 are under development regarding additive manufacturing (Status 03/2021). The first ISO/ASTM standard for AM was published in 2013. CEN/TC 438 on Additive Manufacturing has been working since 2015 to standardize the process of AM. (ISO/TC 261 2020) (CEN/TC 438 2020). Although AM consist currently of only seven processes, entrants and constantly improving systems make it challenging for standards to keep pace.

2.1.1 Additive manufacturing terminology

The EN ISO/ASTM 52900 standard defines nomenclature, terminology, and commonly used acronyms in the additive manufacturing industry. Worldwide acceptance of the term 3D printing as a supersedes term is explained by the fact that it has an analogy with 2D printing on paper, thus being easily understood. The precise definition of the term 3D printing is, making a piece by curing the material using a printhead, nozzle, or other. Usually referring to the low, end level AM devices (EN ISO/ASTM 52900). The use of standardized terminology is particularly justified when new additive manufacturing methods come available and integration into the existing terminology is needed. Technologies such as holography-based 3D printing and volumetric printing are considered as additive manufacturing but are not layer-based. From this point of view, use of the term additive manufacturing is more than justified; it is a neutral umbrella term that describes the subject without commenting on the used manufacturing process itself.

2.1.2 Standardized additive manufacturing processes

The general principle of additive manufacturing is defined in a European standard (EN), current classification and description of the additive manufacturing technologies is (EN ISO/ASTM 52900)

1) Binder jetting (BJT). An additive-manufacturing process in which a liquid bonding agent is selectively deposited to join powder materials.
2) Directed energy deposition (DED). An additive manufacturing process in which focused thermal energy is used to fuse materials by melting as they are being deposited.
3) Material extrusion (MEX). An additive manufacturing process in which material is selectively dispensed through a nozzle or an orifice.
4) Material jetting (MJT). An additive manufacturing process in which droplets of build material are selectively deposited. Example materials include photopolymer and wax
5) Powder bed fusion (PBF). An additive manufacturing process in which thermal energy selectively fuses regions of a powder bed.
6) Sheet lamination (SHL). An additive manufacturing process in which sheets of material are bonded to form an object.
7) Vat photopolymerization (VPP). An additive manufacturing process in which liquid photopolymer in a vat is selectively cured by light-activated polymerization.

EN ISO/ASTM 52900 standard identifies two sub levels of AM, single and multi-step AM processes (Figure 1), based on how many manufacturing phases are required for a finished part.

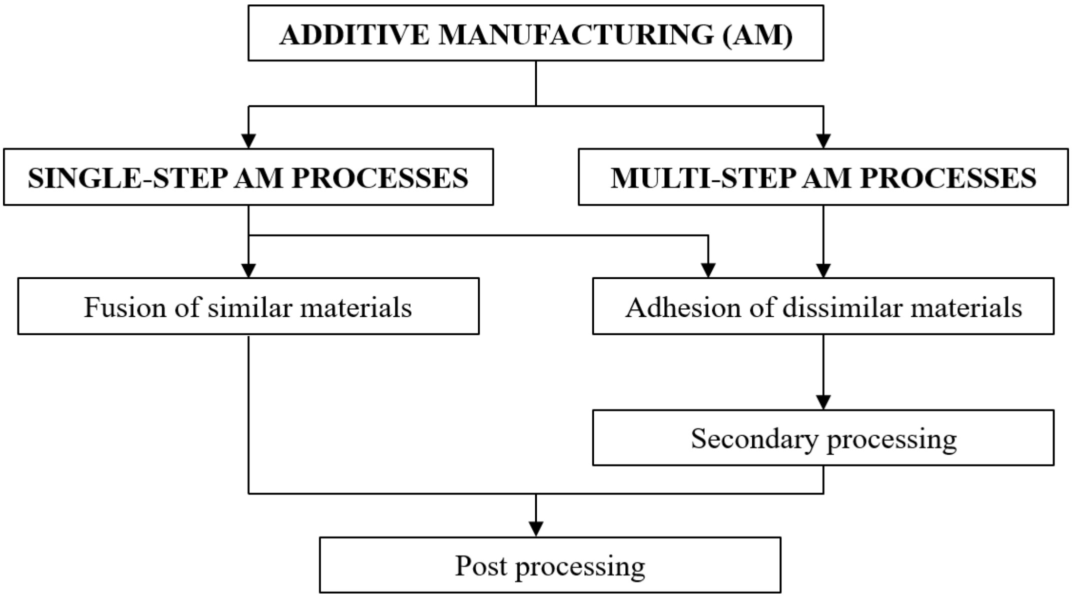

Figure 1. Single-step and multi-step AM processes.

On figure 1, in single step AM process, a part is manufactured through a process where the part obtains its basic geometry and properties directly. Single step AM process is possible for fusion of similar materials. In the case of adhesion of dissimilar materials, or when the part obtains its basic geometry by joining material with a binder but the desired mechanical properties are not yet achieved, secondary processing is required. Despite the process flow, some level of post processing is usually needed for finished parts (EN ISO/ASTM 52900).

2.2 Design for additive manufacturing

Traditionally, when designing a component for a particular manufacturing method, the manufacturing process requirements and limitations must be considered. Additive manufacturing shares similarities with traditional manufacturing methods in this respect. The most significant difference arises from the fundamental way (Figure 2), with which the parts are fabricated. (Diegel et al. 2019, p. 2).

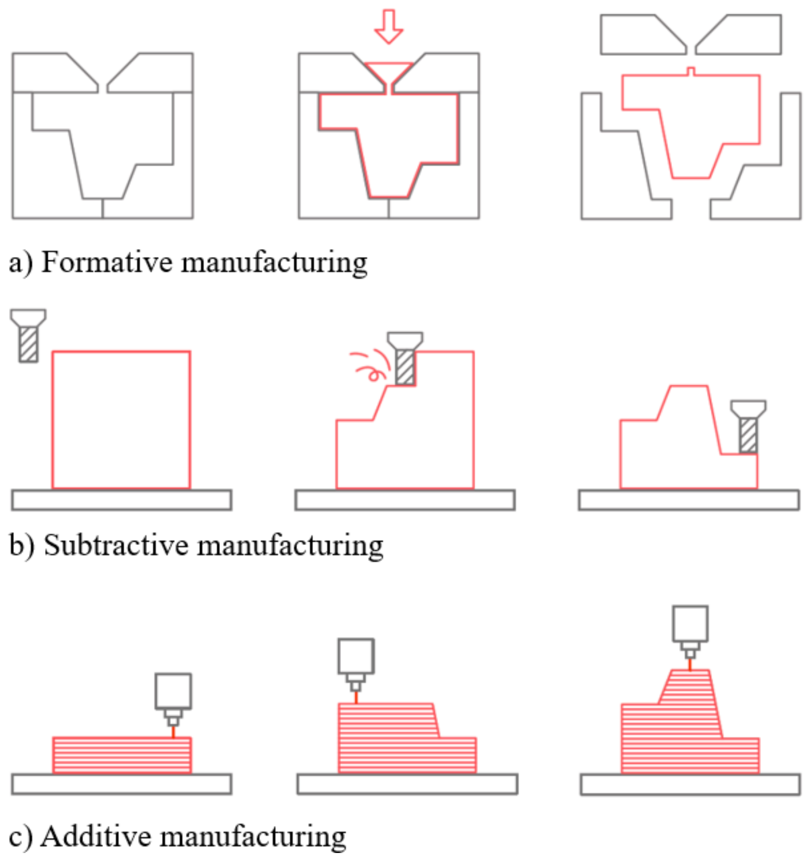

Figure 2. Subtractive manufacturing method (Modified from 3D HUBS. 2021a).

Figure 2 illustrates the formative method a) where a part's geometry restricts its fabrication. The subtractive method b), where a part is fabricated by removing material from the raw piece, is restricted by machinery. With additive manufacturing c), parts are built by connecting volume elements together without any part dependent tools. For example, molds, extrusion dies or milling cutters are not required

Still today, additive manufacturing is too slow and expensive to compete with the conventional manufacturing methods. For this reason, additive manufacturing is usually only used when it is truly adding value to the product. (Diegel et al. 2019, p. 43)

Cost sub-respondent status, quality, manufacturability, and other aspects of AM can be improved by designing the parts specifically to suit AM technology. Design for additive manufacturing (DfAM) is a collection of different tools, methods and strategies that can be applied to take full advantage of the AM technologies. The products must be specifically designed for additive manufacturing. (Diegel et al. 2019, p. 132)

2.2.1 Nature of DfAM

DfAM is a strategy of adjusting part design to make it more suitable to manufacture with additive manufacturing and can be implemented into the design of the product on different levels. Laverne et al. (2015) introduced an idea of distinction between the opportunistic and restrictive natures of DfAM, in other words, design for additive manufacturing can be both enabling and constraining at the same time (Laverne et al. 2015 p. 2). Figure 3 illustrates this.

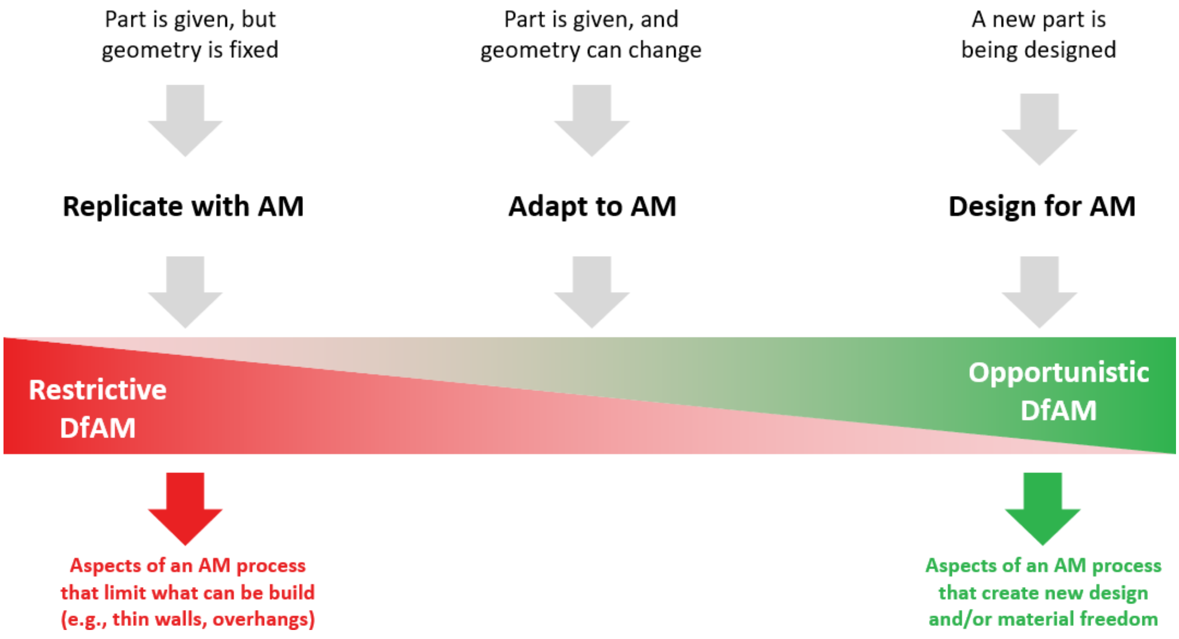

Figure 3. Restrictive and Opportunistic nature of DfAM (Modified from Laverne et al. 2015).

On figure 3, replicate with AM, an existing original part is replaced with a matching AM part, without any redesign, only comprising scanning and printing of the original part as is. The reasoning for using this level of DfAM is when lead-time is enough to justify the use of AM, for example, delivery time of spare parts. On adapt for AM, changes are made to the internal or external form of the part concurrently maintaining the original fit and function of the component. Complete implementation of DfAM is the design for AM, where the entire part is redesigned according to best practices of DfAM. (Diegel et al. 2019, p. 42) Naturally, the DfAM methods are easiest to implement into the completely new fresh design.

The areas where additive manufacturing capabilities are reflected can be summarized as below (Sheng et al. 2015, p. 328), DfAM reflect the same characteristics:

1) Shape complexity: possibility to manufacture practically any shape, which further permits shape optimization.

2) Hierarchical complexity: AM is indifferent against the scale of the details in the part. Micro-structures, surface textures and cellular structures can be fabricated into the same part regardless of the overall size of the part.

3) Material complexity: material can be processed locally, point or layer at a time and selectively. This enables tailored complex material compositions with functional property gradients and structures differentiated by their density.

4) Functional complexity: possibility to integrate different functionalities into the same part.

2.2.2 DfAM process

EN ISO/ASTM 52910 outlines the overall strategy of design for additive manufacturing. It gives requirements, guidelines and recommendations for product design utilizing AM technology. The AM design steps can be structured into three global stages (Vaneker et al. 2020, p. 580):

1) Additive manufacturing suitability exploration
2) Product (re)design for AM Goals
3) Geometry optimization to enable the product realization chain

In general, DfAM should not rely on a set of design guidelines, it should also serve to minimize the technical and economic risks. The complete AM value chain must be considered to evaluate its feasibility, suitability and stability. (Vaneker et al. 2020, p. 581) The first and most important DfAM action is to consider, whether the AM technology should be applied to the product at all. (Diegel et al. 2019, p.580) The most important DfAM tool is the mindset of a designer. The whole AM manufacturing process is very different from the traditional ones, consequently traditional design rules do not apply.

Figures 4 shows a framework chart linking DfAM stages, actions, and goals in relation to the AM design. The framework chart consist of three global design stages that serve to minimize the technical and economic risks before moving on to manufacturing. (Vaneker et al. 2020, p. 581)

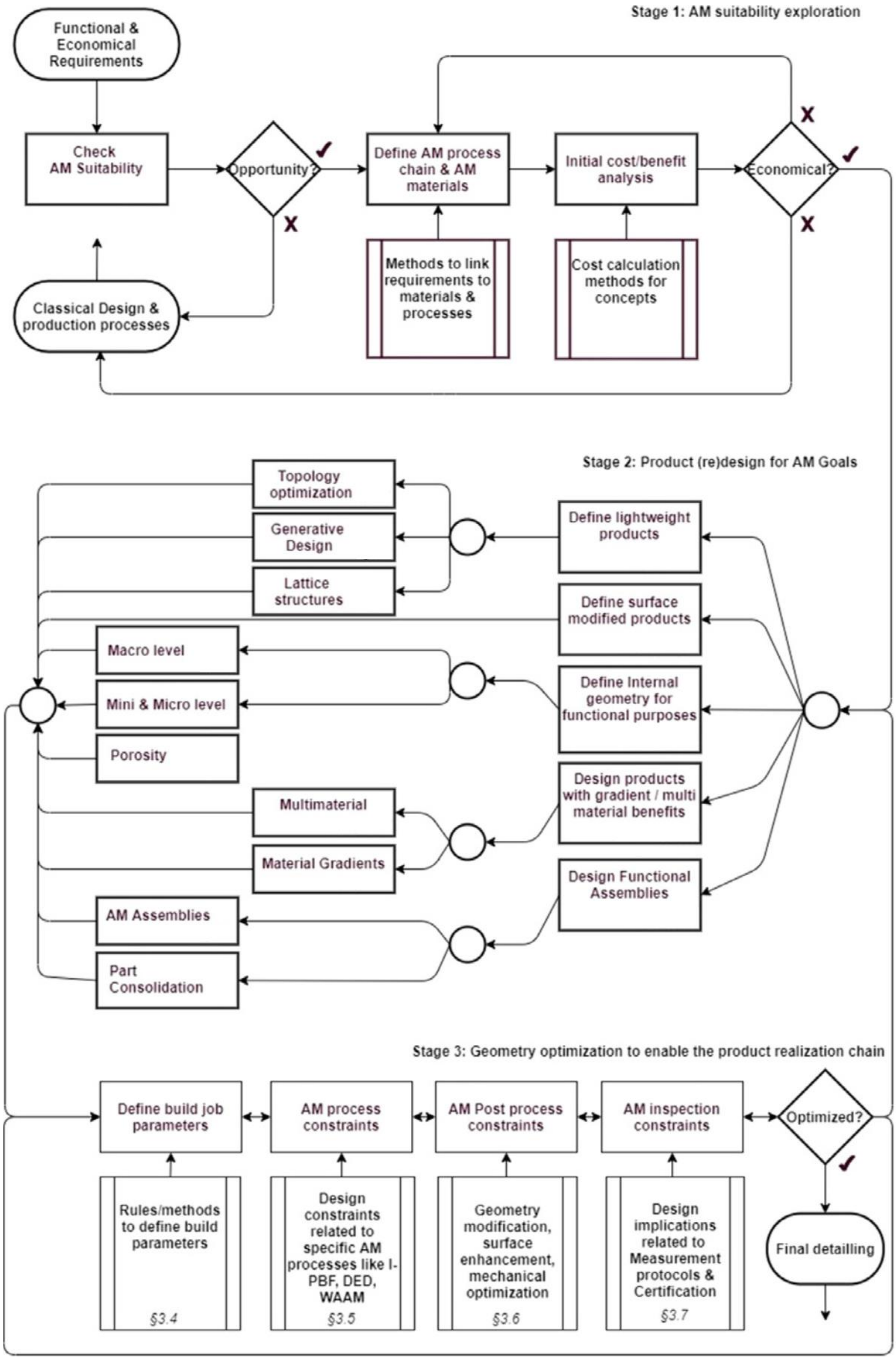

Figure 4. Design framework linking DfAM stages, actions and goals (Vaneker et al. 2020, p. 581).

On figure 4, at stage one, AM suitability exploration, functional and economical requirements of the part to be manufactured are evaluated. Usually, the cost is the primary decision criterion. A criterion may also be functional or technical, quality, delivery time, or any other advantage or product value adding feature which can be achieved with additive manufacturing. Stage 1 is a procedure for identification of general AM potential, if the part is found to be appropriate for AM, the main task at this stage is to find an AM technology and a value chain for the production (Vaneker et al. 2020, p. 581).

The second stage, product (re)design for AM goals, applies all design constrains defined by the initial requirements in stage 1. Design constrains may include factors such as: AM value chain, material, part size, build orientation (if relevant), volume etc. Stage 2 generally consist of different DfAM tools and methods for designing and optimizing part design for the AM process (Vaneker et al. 2020, p. 581). These tools and methods are visited in the following paragraphs.

The third stage is strongly dependent on the selected AM process chain. Stage 3 comprises manufacturing planning, wherein process planning links design and manufacturing. Build job (Figure 4) is a single build cycle in which one or more components are built in the process chamber of the additive manufacturing system. Depending on the AM value chain, aspects like the number of parts produced in single build cycle, build orientation, support structures and post process and quality are considered at stage 3 (Vaneker et al. 2020, p. 581).

2.2.3 Shape optimization

Finding an optimal shape of a component has always been an important objective in engineering, in some sense, all engineering work is optimization: choosing and adjusting design parameters to improve some objective. Computational modelling and optimization algorithms provide a more formal and faster alternative to engineering through trial and error.

Optimization is a field of mathematics and information technology (numerical analysis), which generally examines the problem of finding a solution that is optimal to minimize some cost or objective function while satisfying given restrictions. In the engineering field, optimization seeks material saving, elastic properties, stiffness, strength etc. It can also be applied to the design of optimal flows (electricity, liquid, etc.) in components.

As a mathematical notion, topology is a doctrine of continuity. (Väisälä 2007, p. 6) In the context of topology optimization, topology refers to the material layout or distribution in space. Topology optimization (TO) is a design method that optimizes the material layout within a design space.

Topology optimization has its roots and is a part of structural optimization (SO) wherein optimization problems are formulated to improve structural properties under specified constrains. Objectives are formulated in the objective function with respect to the design parameters. To gain improved objective properties, design parameters must change (Figure 5). Stiffness of the structure and supports beneath the truss represents the constrains. Size, shape, and topology represents the design parameters. The objective is optimal material usage in terms of structural strength (Gebisa & Lemu 2007 p.2).

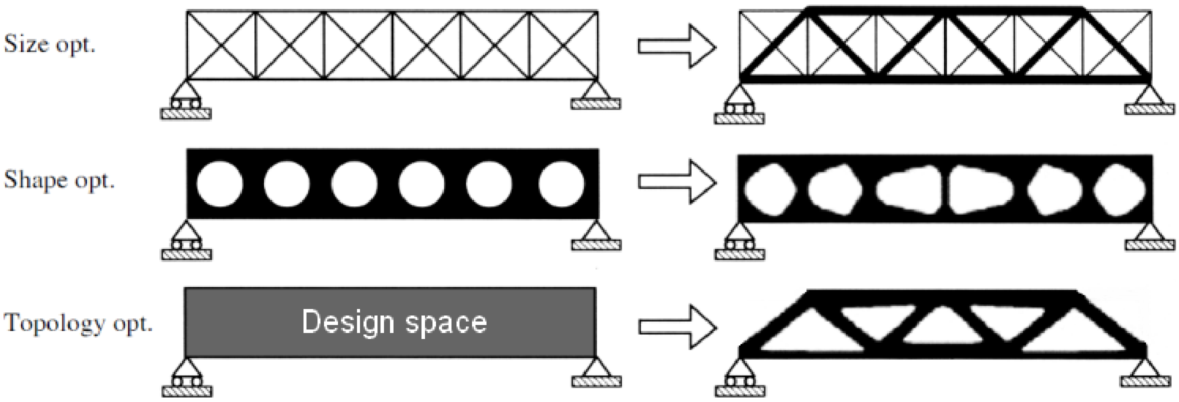

Figure 5. Size, shape, and topology optimization (Modified from Gebisa & Lemu 2007 p.3).

Figure 5 illustrates the fundamental difference of how the design parameters can change. With size and shape optimization, the principal geometry remains the same. With topology optimization, the whole design space is available for editing. Topology optimization combines mathematical and computational techniques to find the optimum material distribution in design space which minimizes or maximizes an objective function.

The numerical method for topology optimization, solid isotropic microstructure with penalisation (SIMP) was originally suggested by Bendsøe M.P. in 1989 on his paper: *Optimal shape design as a material distribution problem*. SIMP is currently the most popular method. One can refer to: An overview on topology optimization methods employed in structural engineering, to extend the idea about the subject (Yuksel 2019).

The shape obtained as a result of topology optimization is characterized by a strong organic nature (Figure 6) resulting in difficult to manufacture geometries with traditional methods. Thus, topology optimization being a perfect match for additive manufacturing.

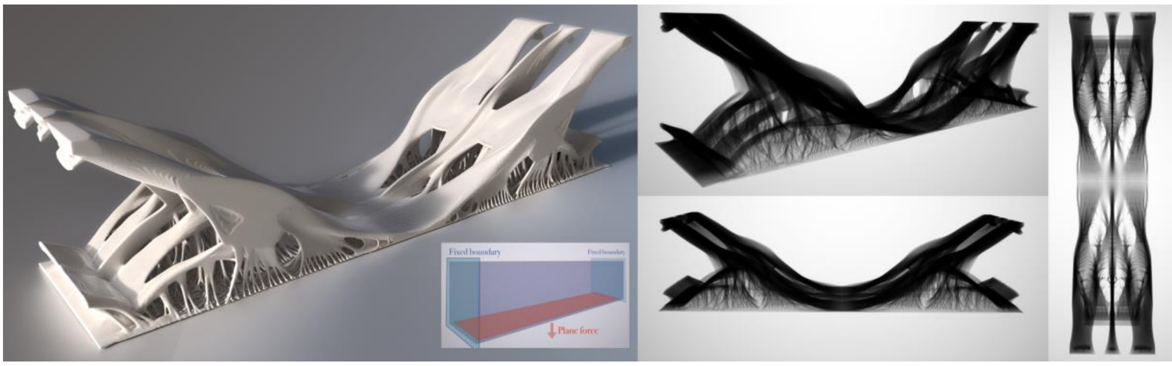

Figure 6. High-resolution, Narrow-Band Topology Optimized bridge structure (Liu et al. 2019 p.4).

Figure 6 illustrates an optimized bridge like structure constructed by high-resolution narrow-band topology optimization method. X-ray-like images on the right visualizes the material density field.

The main application of topology optimization for additive manufacturing has been to reduce the cost of parts through material use and build time, in respect to the optimal strength. General TO application uses finite element analysis (FEA) to evaluate design performance. In the process, TO algorithms together with the FEA are used to determine which areas or volumes are not crucial in terms of the desired objective and can be removed. Topology optimization can solve several physical phenomena related engineering problems, optimal material distribution against strength being the most common application. In addition to this, it is reported in several research papers how TO is utilized to create added value on additive manufactured parts, such as negative poisson’s ratio, negative thermal expansion, optimized thermal convection and fluid flow, as a few examples. (Sigmund)

2.2.4 Computational fluid dynamics driven topology optimization

Although the topology optimization method gained maturity within structural optimization and optimal strength as an objective, the TO method has since been extended to a wide range of physics. Computational fluid dynamics (CFD) is a component of flow mechanics in which numerical methods are used to solve and analyze the behavior of fluids, i.e., liquids and gases (Figure 7). The aim of the CFD driven topology optimization is to optimize part geometry for fluid flow efficiency.

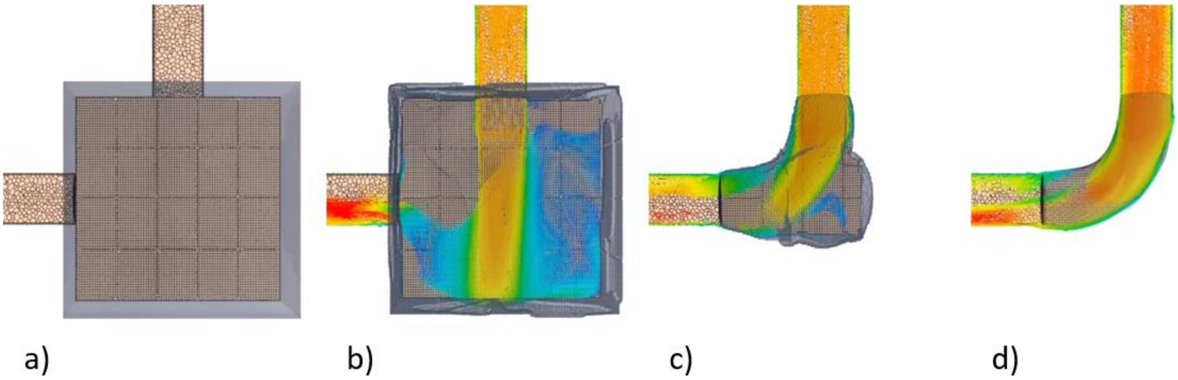

Figure 7. CFD driven topology optimization process (Modified from Siemens 2021).

Figure 7 illustrates the CFD driven topology optimization process. Although there are other methods, CFD driven topology optimization comprises a three-dimensional design space (a) which defines the geometric boundaries for the solution. The optimization process is carried out on a computational mesh where a single mesh cell is considered as a design variable. During the optimization run, an optimization algorithm iteratively suppresses the flow on a cell-by-cell basis (a-c) until no significant changes in the flow sedimentation occur in respect to optimization objective (d) (Siemens 2021).

CFD is not limited to the flow of liquids and gases. Figure 8. illustrates the thermal conductivity optimization of a heat sink.

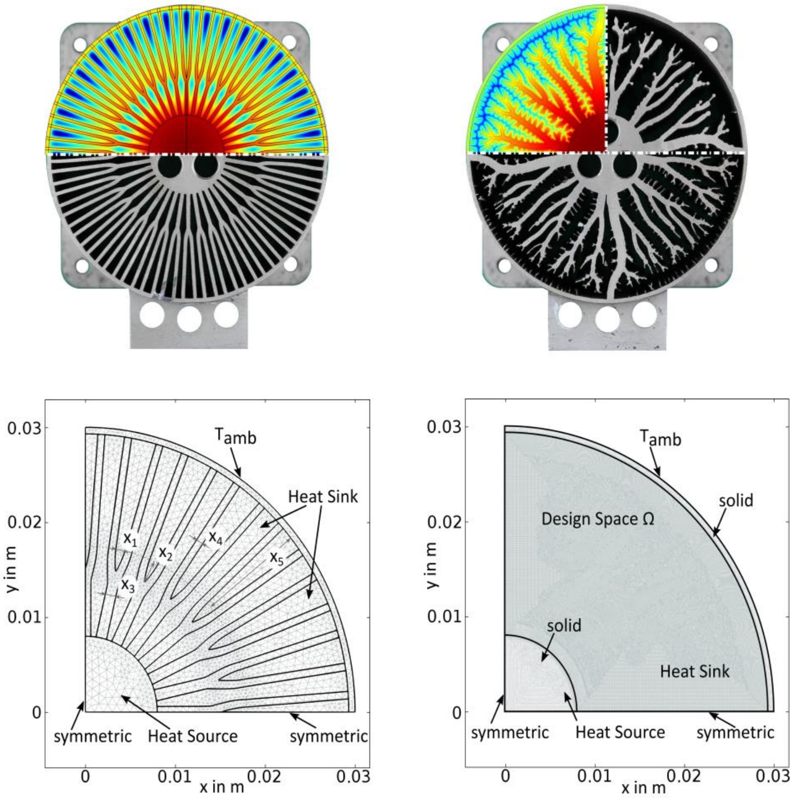

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Figure 8. Comparison of parametric and topology optimization (Modified from Lange et al. 2018) .

Figure 8 shows a comparison between the parametric and topology optimization methods. Parametric optimization (left) is limited to strict boundary conditions, such as the number and shape of the fins (bottom left X1-X4.) The topology optimization method has a whole design space for editing (right). Lange et al. (2018) concluded that the topological optimum offers a better thermal resistance in relation to weight than the conventional component.

While organic geometry created through the topology optimization process lead to increases in performance, the designs created are rarely useful as such, especially for traditional manufacturing methods. For AM, models resulting from optimization need to be smoothed into more printable geometrises. This can be done programmatically or by reworking the whole geometry and only taking the TO design as an idea for the optimal geometry (Diegel et al. 2019, pp. 68-70).

2.2.5 Generative design

Generative design (GD) is not generally considered as an essential DfAM method, although it has a clear connection to additive manufacturing in terms of the manufacturability of the parts. Generative design has its roots in architecture and civil engineering, where the method has been used for optimizing, for example, building floor space, layout, availability of natural light in the office or the views of a nearby beach. Instead of making several design iterations or concepts manually, generative programs can produce and solve optimal design proposals. Generative design embodies the design process. The core of the generative design methodology is how artificial intelligence (AI) algorithms are utilized to give and help designers explore different design options and make informed decisions (Autodesk Revit 2021).

The terms generative design and topology optimization are used interchangeably, this confusion is probably because both techniques produce very similar organic results and the inputs, loads, constrains etc. to generative design are similar with the inputs to topology optimization. Generative design differs from topology optimization in the way, where TO takes a design space and seeks optimal material distribution under given constrains converging on a single solution, GD processes all possible solutions using artificial intelligence and topology optimization algorithms to produce multiple solutions (Figure 9). In this sense, TO is a foundation technology upon which GD is build. (Briard et al. 2020, p.878)

Figure 9. Multiple design solutions of the same part (Modified from ADSK NEWS 2021).

Figure 9 examples a case, where the GD software generated 150 valid design options, 8 initial components were consolidated into one, and the new solution was 40% lighter and 20% stronger (ADSK NEWS 2021).

Generative inputs are information of design constrains, forces, materials, cost etc. that the GD program will respect and target during the generative process. Generative inputs may include manufacturing constraints, meaning that GD will consider the practical needs of a certain manufacturing method. From DfAM's point of view, GD is a tool that can be used to ensure manufacturability of the AM part.

Briard et al. (2020) investigated how to include generative design in the design for additive manufacturing. They ended up proposing a new design methodology G-DfAM, a generative design workflow to design additive manufactured parts using generative design tools.

2.2.6 Lattice structures

Porosity refers to the portion of an object that is not solid. Multiple examples of porous objects can be found in nature, where evolution has created strong, and at the same time light structures. The honeycomb structure being perhaps the best known. Techniques to achieve porosity in additive manufacturing are lattice and infill structures.

In additive manufacturing, lattice structures are used to reduce material, build time and energy utilized in the manufacturing process, simultaneously maintaining part strength while minimizing the weight. (Helou Kara 2018 p. 243) In addition to this, lattice structures are beneficial as they can be constructed for specific structural properties. Lattice structures are widely used for energy, acoustic and vibrational absorption.

Due to the differences in AM methods, DfAM refers herein to the ease of fabricating lattice structures with the AM technology used. Lattice structures are expected to be fabricated without support and be self-supporting. However, AM parts are built layer by layer and in the case of missing contact or contact being too small with the previous layer, support structures are needed. Herein selective laser sintering (SLS) process has a competitive edge over other processes, since in it, bed powder can act as a support material. The practical problem is to remove the powder from inside the lattice structure (Wenjin & Ming 2016, p.326).

The shape, size, and topology of lattice structures varies greatly. Therefore, there is no unified concept about the definition of lattice structures. In this thesis, the same definition is used as in Pan et al. 2020: “Lattice structure is a porous three-dimensional spatial structure formed and tessellated by unit cells with different topological geometries, and belongs to cellular structures (including foam structure, honeycomb structure and lattice structure)”

Despite the confusion with the terminology, a unit cell (Figure 10) is the basic, smallest seed unit which is repeated over the domain to construct a lattice structure.

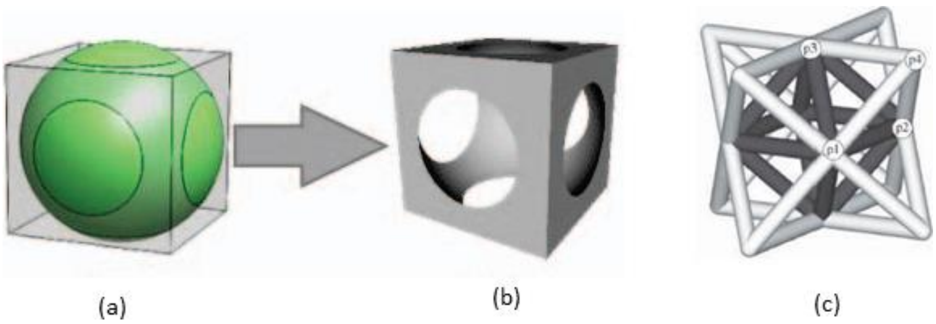

Figure 10. Primitive based unit cells (Modified from Wenjin & Ming 2016, p.327).

Figure 10 illustrates different approaches to construct a single unit cell. The primitive based method (a,b), where the unit cell is constructed from basic primitive geometries with Boolean operations, or from beams and truss features (c) with nodes to create transitions and connections between unit cells. (Pan et al. 2020, p. 4) (Pan et al. 2020, p.249)

The implicit surface method, also referred to as a mathematically generated unit cell or a formula-driven lattice, is a method where implicit equations are used to represent the surface of the unit cell. One of the methods to transform a mathematical model into a lattice structure is triply periodic minimal surface (TPMS) (Figure 11) By definition, TPMS is the minimal surface for a given boundary. Meaning that the surface locally minimizes its area while it splits the space inside the boundaries into two or more domains. (Al-Ketan et al. 2019a, p.2)

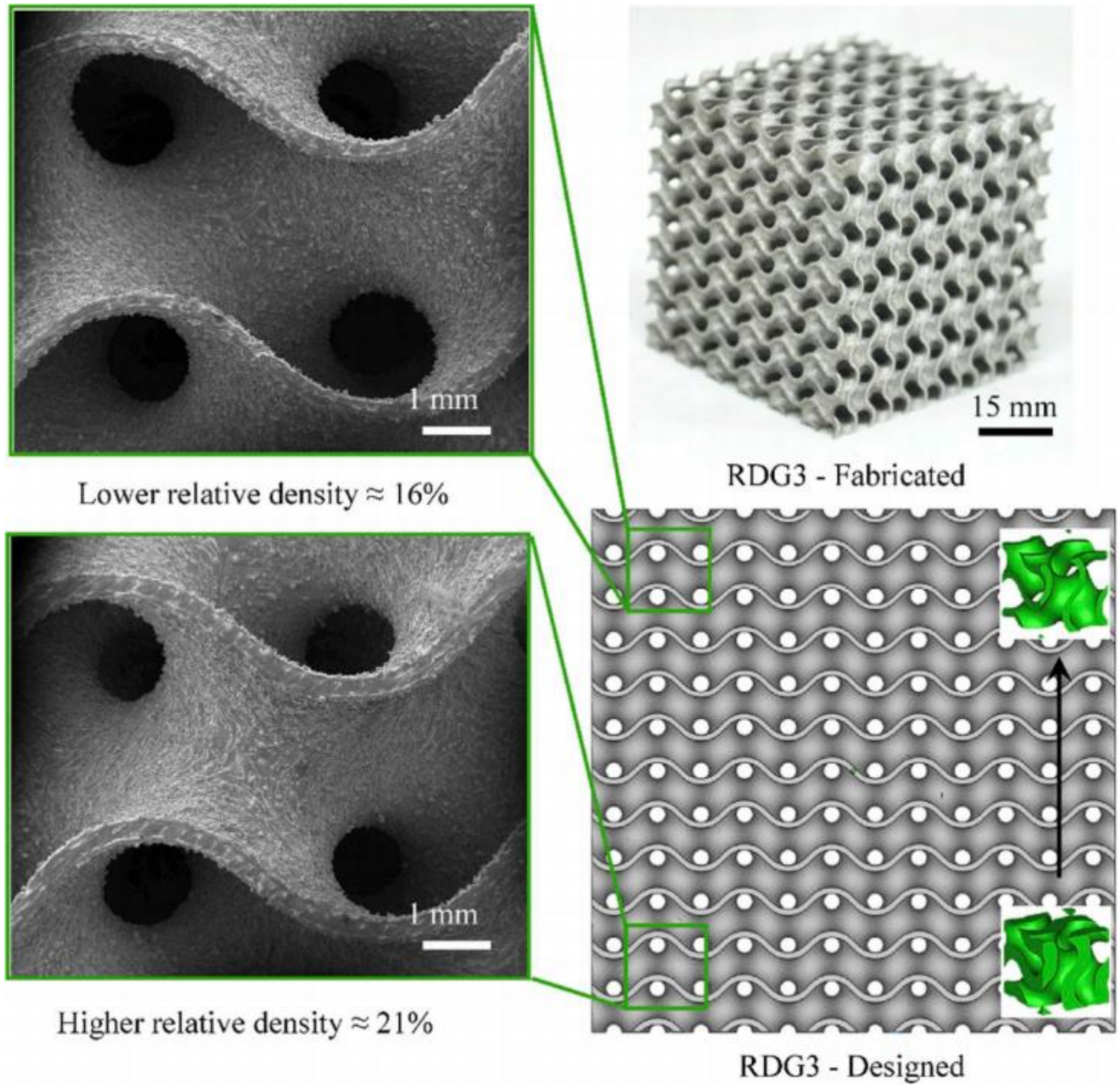

Figure 11. AM manufactured lattices with relative density grading TPMS unit cell (Al-Ketan et al. 2019b, p. 7).

Figure 11 shows a variable density lattice structure constructed by TPMS surfaces. Due to its unique geometry, TPMS lattice structures has several advantages compared to primitive based unit cells. It has a high surface-to-volume ratio, smooth surface and transition, it is not prone to stress concentration, and due to the mathematical expression of a unit cell, a variable-density cellular structure is easy to generate. In addition, TPMS geometry can be self-supporting if orientated correctly (PTC 2021).

One of the simplest ways of populating design space with a lattice structure is by patterning (repeating) unit cells over the design space while maintaining size, shape, and orientation of the seed unit cell, resulting in a linear array of unit cells. A more sophisticated method is conformal patterning (Figure 12).

Figure 12. Conformal populating of lattice structure (Fast radius 2021).

Figure 12 shows a conformal lattice structure, where the populating of shape varying unit cells is controlled to follow the initial three-dimensional shape of the design space.

Non-uniform lattice structures can be constructed manually, parametrically or via topology optimization to meet specific performance by adjusting unit cell characteristics and lattice density (Pan et al. 2020 p. 17). Non-uniform lattice structures have variable density and porosity and can combine a variety of different unit cells shape characteristics. Compared to uniform lattice structures, non-uniform lattice structures enable more free design and can be optimized to meet the needs of practical application. Variating porosity and irregularity influence the mechanical properties of the material. Characteristics such as elastic moduli, permeability, thermal expansion rate and conduction can be optimized (Pan et al. 2020, p. 9).

2.2.7 Part consolidation

Design for manufacturing and assembly (DFMA), is a design methodology for traditional manufacturing. DFMA is defined as a practice of designing products to minimize manufacturing and assembly difficulties and costs. In design for assembly, two main means of assembly facilitating are reducing the number of parts and eliminate fasteners, since the number of assembly operations is the primary driver for assembly cost. Assembly facilitating is usually achieved by integrating individual components into one, what in turn increases the component complexity and manufacturing cost. In most cases, combining different functionalities into one part requires the usage of advanced manufacturing methods.

For AM, a similar assembly facilitating method is part consolidation, where a component is designed to fulfill shape and functional requirements while still being manufactured as only one physical body. Figure 13 shows a hydraulic primary flight control component of Airbus A380, AM manufactured by Liebherr-Aerospace.

Figure 13. Part consolidated Airbus A380 valve block (Liebherr 2021).

Figure 13 illustrates a part consolidation solution where the hydraulic fluid channels and a valve body are directly connected to each other. This avoids the need for a complex system of pipes and transverse bores, thus saving time in production. (Liebherr 2021).

2.3 Energetic materials

Energetic materials are substances which store a large amount of chemical energy that can be released rapidly. While combustion is generally associated to take place between a burning substance and atmospheric oxygen, energetic materials can contain all the oxygen or other reactants necessary for their combustion. Energetic materials are capable of a dual reacting regime, supersonic detonation regime and subsonic deflagration regime. The difference between detonation and deflagration lies only in the reaction velocity. In detonation, the reaction propagates at supersonic velocity, in deflagration, the reaction velocity is relativity slow, subsonic (Akhavan 2004, Pp. 60-61). Both are methods by which energy is released, and when controlled, can be harnessed to do work.

2.3.1 Manufacturing of energetic materials

Products made of energetic materials are usually manufactured by casting, pressing or by extrusion. In the casting process, the molten material is poured into a container and solidified by cooling in controlled conditions. In the pressing process, the material is pressed into a container and in an extrusion method, pushed through a die of the desired cross-section (Akhavan 2004, pp. 156-161). These traditional manufacturing methods represent the formative manufacturing approach and are therefore relatively limited methods in terms of shape complexity. In addition, post processing is required to obtain a final shape. Post processing may include cutting, milling and sawing. (Akhavan 2004, p158)

2.3.2 Detonation

An explosion occurs when a large amount of energy is released in short order. An explosion may occur from a rapid physical transformation of the state, such as pressure vessel failure, or from a rapid exothermic chemical reaction resulting in a large amount of heat and gas. (Akhavan 2004, p.21) Detonation refers to a rapid and violent combustion, involving a supersonic exothermic detonation wave accelerating through an explosive medium. Detonating substances are materials that can rapidly decompose through the effect of shock wave propagation (Akhavan 2004, p. 64).

Detonation theories, for example, the Zeldovich-Neumann-Doering (ZND) theory, models the detonative combustion and explains the internal structure and propagation mechanism of the shock wave (Davis & Fauquignon 1995, p.13). The shock wave compresses and heats the material during its propagation and the released energy in turn assists in sustaining the pressure of the shock (Figure 14).

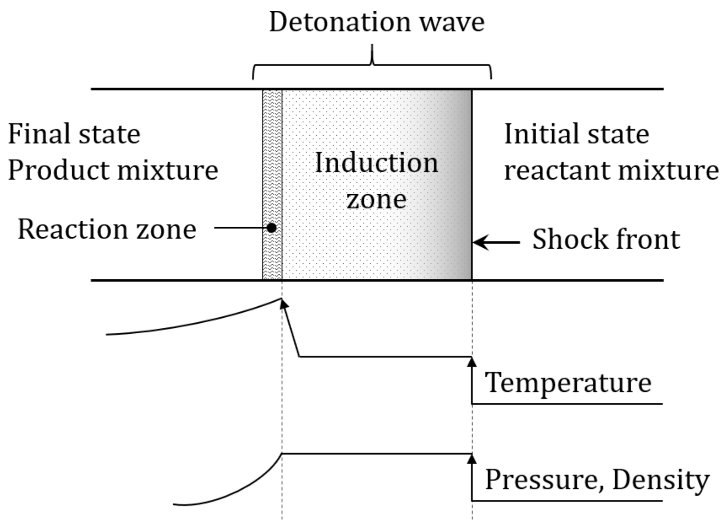

Figure 14. A ZND detonation model diagram showing the pressure, temperature and density profiles of the propagating shock wave.

Figure 14 shows a schematic diagram of the ZND model including pressure, temperature, and density profiles. The ZND model comprises of a planar shock front, followed by a nearly thermally inactive induction zone where a detonative substance decomposes and forms reactants. A rapid exothermic reaction occurs in the reaction zone resulting in temperature rise while pressure and density decrease as reaction product gases expand. The propagation mechanism of the shock wave is explained in the ZND model with the expansion of reaction products. During exothermic reactions in the reaction zone, the reaction product is heated and expands providing amplification and support to the forward propagating shock wave. In turn, an upstream propagating shock wave processes more reactive material in front to fuel itself (Akhavan 2004, p.72).

2.3.3 Deflagration

Deflagration of energetic materials differs from traditional combustion (burning) and detonation in terms of reaction velocity. Since the presence of atmospheric oxygen is not needed for the reaction of energetic materials, the velocity at which deflagration propagates depends upon the reactivity of available reactants and therefore is faster and more violent than ordinary combustion, reaction still being slower than detonation, subsonic. (Akhavan 2004, Pp. 60-64), This is also a basis for how explosives are categorized as detonating high explosives (HE) and deflagrating low explosives (LE).

The difference between combustion (burning) and deflagration is also in the ignition and propagation mechanisms. Whereas thermal energy generated during combustion reaches the substance at the rate of oxidation, ignition and propagation of deflagration occurs through hotspots that cause a sequence of reactions to commence. Once simulated by external energy, heated hotspots trigger self-sustaining combustion in nearby substance. Externally simulated hotspots may be caused through friction, compression, heat, percussion, impact etc. In addition, a failed detonation can fade to deflagration (Akhavan 2004, pp. 50-51, 64-67).

2.3.4 Blast wave

A pressure wave is a pressure difference propagating longitudinal in a medium that can be treated as a fluid. In kinematic terms, longitudinal propagating pressure waves are also referred to as compression waves since the basic characteristics of longitudinal waves are the compression and rarefaction of the medium parallel to the direction of wave propagation, traveling away from the source (P-Wave 2021).

Blast waves are associated with supersonic detonations. If the energy release from the source is sufficient, the rate of the deposited energy exceeds the ambient sound speed and a longitudinal propagating pressure wave manifests itself as a propagating disturbance shock front (Needham 2018, p. 8). An ideal blast wave profile is commonly presented with the Friedlander plot (Figure 15) which presents the pressure (P) in function of time P(t).

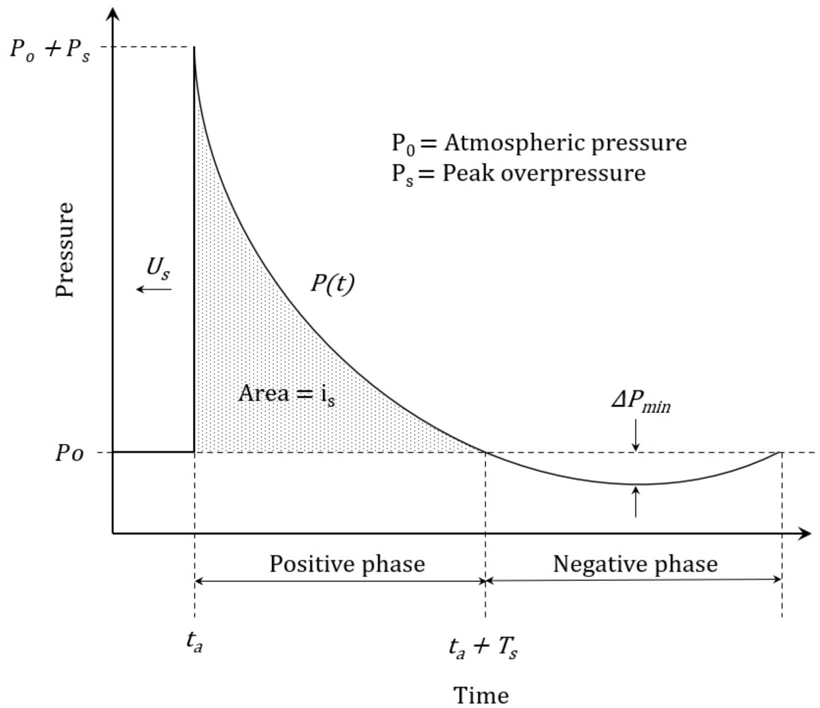

Figure 15. Ideal blast wave presented with the Friedlander plot

Figure 15 illustrates an ideal air blast wave's pressure development over time measured from a distance. Area I_s is a measure of energy from a detonation, a more common method to express the blast wave energy is in terms of the equivalent weight of TNT (Needham, C. 2018. pp. 54-56). The pressure profile of deflagration is calmer and differs in peak pressure, duration of the impulse and in decrease of overpressure.

2.3.5 Affecting factors on blast pressure distribution.

The effects of overall aspect ratio, shape, and the location of an initiation point are as important to the dynamics of the generated pressure as the chemical composition or mass of the EM product. (Simoens B. & Lefebvre M. 2015 p. 195) Already in 1792, German mining engineer Franz Xaver von Baader, proposed the adoption of a conical or mushroom shaped cavity at the forward end of the blasting charge to increase its efficacy and to save powder. A later invention, Charles E. Munroe’s lined cavity principle which dates to 1888, also applies a blast wave focusing effect but its metal piercing ability (Figure 16) is based on the kinetic energy of a metal liner in front of the cavity (Kennedy D. 1990 pp. 5-6)

Figure 16. Munroe cutting effect (Modified from Scopex 2021 and Smith J. 1984).

Figure 16 illustrates the Munroe effect used for the cutting of a metallic structure by focusing and changing the direction of detonation wave propagation.

To determine the effects of shapes on pressure distribution, the L/D aspect ratio has been the main area of interest in literature. Artero-Guerrero J. et al. (2017) developed a numerical model to analyse the influence of basic shapes with different aspect ratios and Simoens B. & Lefebvre M. (2015) carried out experiments to quantify the shape effect for different L/D ratios, a few to mention. An effect of the L/D relationship is illustrated in figure 18 from measurement data.

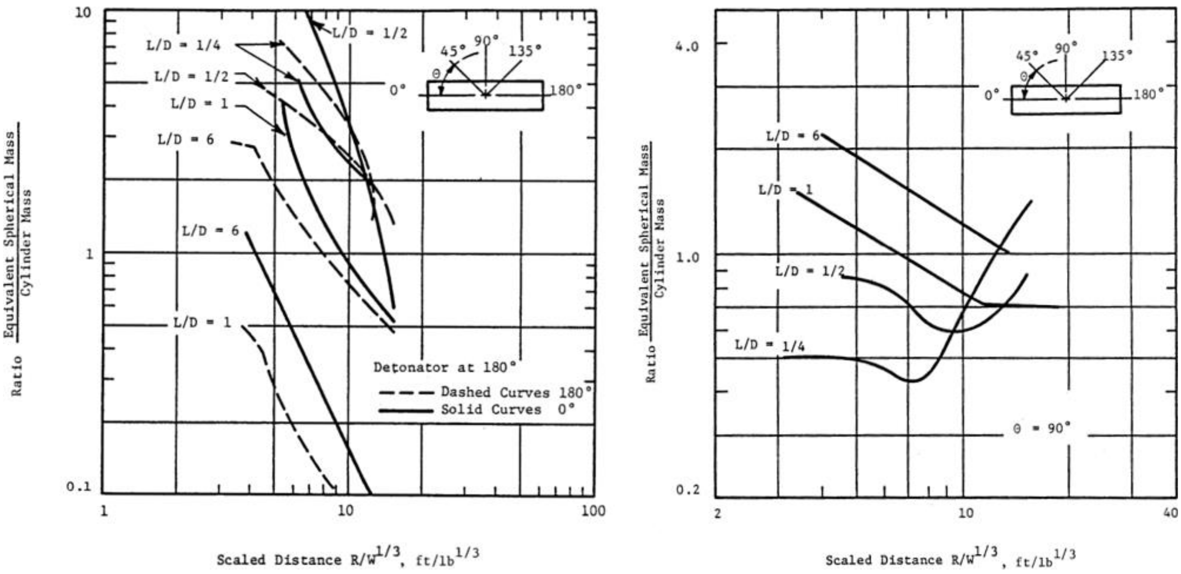

Figure 17. Empirical relationships for cylinders with various L/D ratios at θ = 0° and 90° (Modified from United States Department of Energy. 1980, p. 4-62…63).

Figure 17 shows a blast wave pressure distribution from a cylindrical shaped source. L is the length and D is the diameter. Pressure histories depend on the aspect ratio L/D so that a larger aspect ratio (>1) directs the energy in radial 90° direction whereas smaller ratios in axial 0° direction. The L/D ratio for an optimal radial pressure is 6/1 (Knock C. & Davies N. 2013 p.337-338).

The velocity of detonation will increase as the diameter increases up to a certain limit value, still the diameter of the cylindrical shape cannot be exploited indefinitely. The shock wave front shape for a cylindrical shaped pellet is convex rather than ideally flat and diminishing from the centre to the surface. The critical value for a diameter where the surface effect disturbs and destabilizes the shock wave is referred to as the critical diameter (Akhavan 2004, pp. 70-71).

The direction of the greatest pressure corresponds to the largest surface area of the source. Knock C. & Davies N. 2013 p.338) Table 1 shows a measured pressure shape amplification ratio compared to the reference spherical source. Amplification ratios presented in the table are determined by dividing the pressure from different shapes and angles by the pressure for the sphere. The angles are the same as in figure 22.

Table 1. Comparison pressures ratio relative to spherical shape (Johnson C. et al. 2018, p.4)

Ratio	**Near Field**			**Far Field**		
	Primary Wave Facet (90 -Degrees)	Bridge Wave Vertices (135 -Degrees)	Primary Wave Facet (180 -Degrees)	Primary Wave Facet (90 -Degrees)	Bridge Wave Vertices (135 -Degrees)	Primary Wave Facet (180 -Degrees)
$P_{Cylinder}/P_S$	**1.31**	1.1	0.46	1.01	**1.08**	1.04
P_{Cube}/P_S	**1.26**	1.04	**1.37**	0.76	**1.19**	0.76
$P_{Tetrahedron}/P_S$	**1.26**	0.96	**1.26**	0.98	**1.16**	0.77

Table 1 shows, that where a cylinder shaped source directs the energy mostly in radial 90° direction in the near field, planar surface shapes (facet) also direct the energy in a similar fashion. In the far field, the pressure equalizes spherically. The rise in pressure at the far field is explained by the effect of a bridge wave. (Johnson C. et al. 2018 p.4)

Many articles dealing with the dynamics of the generated pressure waves concern only basic geometrical shapes. In the near field to the source, it has been shown, that different geometry configurations influence the pressure distribution (Artero-Guerrero J. et al. 2017 p.197) (Simoens B. & Lefebvre M. 2015 p. 221)

The performance of energetic materials is not dependent only on the chemical composition of the substance. Energetic materials create heat and gas through a surface reaction. The velocity of the reaction increases as the substance compaction density and degree of confinement increase. Velocity of detonation (VOD) indicates the performance and propagation of chemical decomposition (Akhavan J. 2004, Pp. 68-69).

The velocity that the deflagration front progresses at is known as the linear burning rate, defining the rate at which a mass of substance is turned into reaction products. Being a surface reaction, the surface area involved in the reaction affects the amount of material reacting at the surface area in unit time. The amount of substance consumed in unit time depends upon its density, reaction surface area and burning rate. The rate at which the detonative material decomposes depends upon the speed at which the material transmits the shockwave (Akhavan J. 2004, Pp. 62-64).

The modern configuration of an energetic device consists of a more sensitive initiator and a less sensitive but more powerful main substance. This arrangement is aimed at the security and prevention of unintended initiation and is achieved with various additives (Akhavan J. 2004, Pp. 82). The use of additives offers an extended range of performance, but a similar effect can be achieved with compositions with inert granular inclusions (voids). Anshits A. et al. (2005) investigated the detonation velocity and critical diameter of an emulsion explosive containing 50-250µm microspheres and 70-100 µm cenospheres and noticed a reduced initiation sensitivity. Herring S. et al. (2010) simulated the effects of various arrangements of circular voids.

By combining two or more substances with different detonation velocities and suitable interface geometries, blast energy direction and anisotropy can be altered. The analogy between detonation dynamics and geometric optics is presented in figure 18.

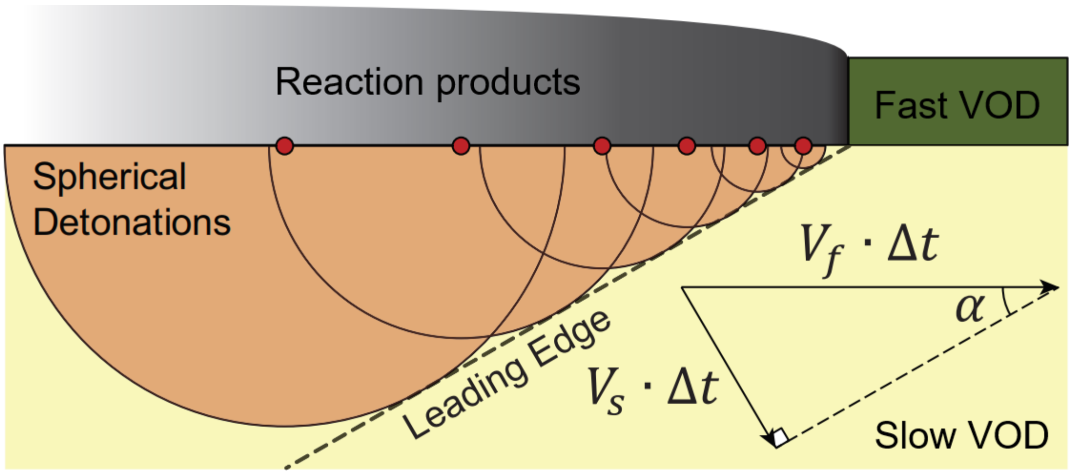

Figure 18. Formation of a tilted shock wave (Modified from Loiseau J. et al. 2014 p.2).

Figure 18 shows a tilted shock wave in the slow VOD substance conceptually identical to Huygens' principle. According to Huygens' second principle, the new position of a wave front is the sum of wavelets emitted from all points of the wave front in the previous position. Each fast VOD point source expands spherically with a velocity equal to the slow VOD resulting in a shock wave tilted by an angle α (Loiseau J. et al. 2014). Experiments have shown that shock energy can be altered by converging shock waves (Pacsci emc. 2021). In figure 20 the interface between two different VODs is straight. With additive manufacturing an arbitrary complex shape would be possible.

2.4 Printability considerations of energetic materials

Although several research papers are available for the additive manufacturing process, not so many were found concerning particularly the additive manufacturing of energetic materials and their applications. Muravyev et al. (2019) reviewed additive manufacturing methods for energetic materials and potential applications for printable reactive microstructures. Woods H. et al. (2020) investigated the rheological properties of energetic materials by experimental methods and Castellanos J. et al. (2019) investigated the printability of an ammonium perchlorate composite propellant. Van Driel C. et al. (2017) gives a presumably state of the art outlook for developments in additive manufacturing of energetic materials. Additive manufacturing methods applied to energetic materials are presented in figure 19. (Muravyev et al. 2019 p.942)

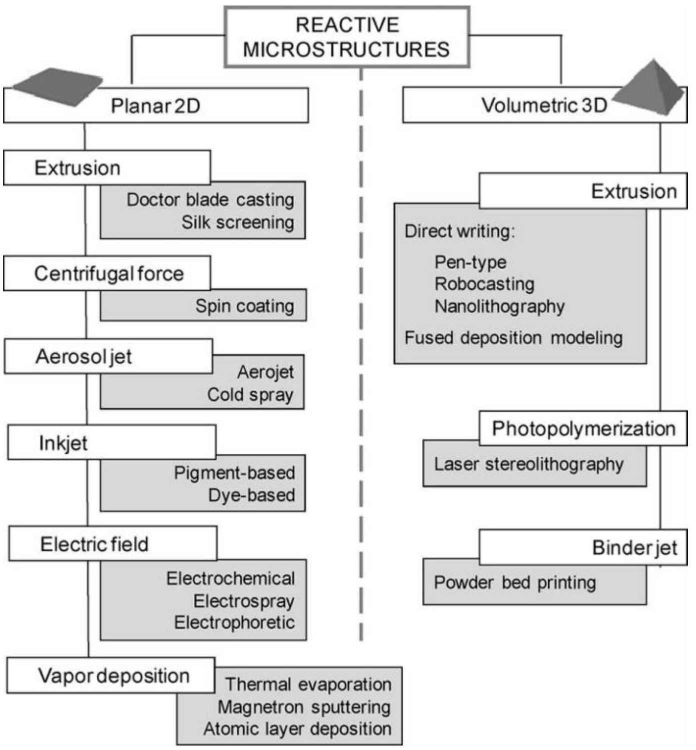

Figure 19. Additive manufacturing methods for reactive microstructure fabrication (Muravyev et al. 2019 p.942).

On figure 19, the extrusion methods refer to the standard EN ISO/ASTM 52900 material extrusion (MEX) additive manufacturing process in which material is selectively dispensed through a nozzle. In practice, DIW, FDM etc. differs only in terms of material supply and state. The point of interest in this thesis is the direct ink writing method (Figure 20).

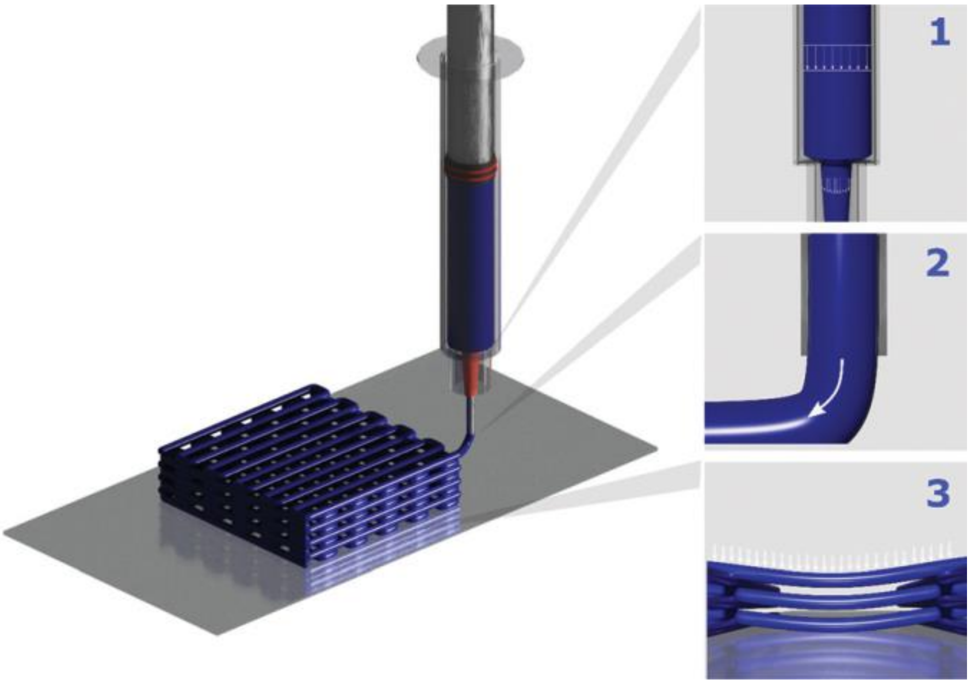

Figure 20. DIW deposition process (Modified from Tagliaferri et al. 2021 p.542).

Figure 20 illustrates the principle of continuous direct ink writing printing process. The same principle applies to all MEX processes. DIW is an extrusion based method where viscoelastic paste “ink” is stored in a syringe barrel or container (1), extruded through a nozzle (2) and deposited along a path to fabricate a 3D object layer by layer (3). Material flow is generally generated by the action of a pump, piston, air pressure or Archimedes’ screw.

DIW has the potential for the fabrication with a great accuracy. The ability to extrude filaments at room temperature without the interfering effect of heat, features smaller than 1 µm can be printed. (Tagliaferri et al. 2021 p.541) Instead of heating the material over its melting point to obtain viscoelastic behaviour, as in the FDM process with thermoplastic materials, the extrusion and solidification of material in the DIW process relies on the rheological properties of the material. Rheology is the branch of physics which studies the way how materials deform or flow in response to applied forces or stresses.

2.4.1 Rheology

For a successful printing process, knowing the material behaviour and properties initially is mandatory. AM process specific parameters and such are adjusted according to the material, which is homogeneous by default. This is common practice also for other MEX processes, for example in the MEX-FDM process, the nozzle temperature varies according to the used material. From the DfAM perspective, the DIW process is opportune if the ink can be extruded in a form of a continuous filament and the desired geometry is archived. To obtain this, control over the rheology of the ink material is fundamental since it has a direct link with printability, while the nozzle diameter is a main factor that influences print resolution. Well printable ink flows smoothly as a continuous material flow without jamming the deposition nozzle. This directly depends on the viscosity of the material (Figure 21).

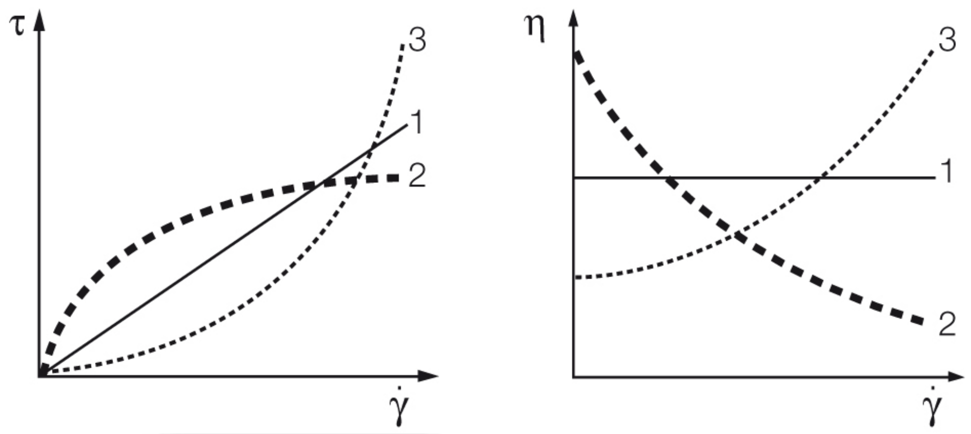

Figure 21. Flow curves (left) and viscosity curves (right) for (1) ideally viscous, (2) shear-thinning, and (3) shear-thickening flow behaviour.

Figure 21 illustrates Newtonian and non-Newtonian viscosity behaviours. Shear rate $\dot{\gamma}$ is the rate at which shearing deformation is applied to the material. At Newtonian viscosity behaviour (1) viscosity η is independent of shear rate and is constant. If the fluid's viscosity depends on shear rate and shear stress τ, it can be shear thinning (3) or shear thickening (2) a.k.a. non-Newtonian viscosity.

Shear thinning (or pseudoplastic flow) behaviour of materials whose viscosity decreases as the shear rate increases, is usually sought to meet the flow criterion and employed in the DIW process (Tagliaferri et al. 2021 p.541). This is achieved because the printing material is affected by the shear stress during extrusion through a nozzle. Another approach is to use low viscosity ink and solidify the material by other means, such as the precipitation of a binder, solvent evaporation, gelation or by radiation curable material. In addition, high-amplitude ultrasonic actuators are used to reduce nozzle friction and improve the flow rate significantly. (Muravyev N. et al. 2019 p.951) Literature gives a wide, substance composition specific viscosity range for an ideal shear thinning ink. For example, printed polymers require a viscosity between 0.3 Pa·s and 100 Pa·s. Between these limits, the ink maintains a desired shape after extrusion without clotting the nozzle. (Casanova-Batlle E et al. 2021 p.2)

The general character of shear thinning fluids is that they can flow only if they are submitted to a shear stress (Figure 22) above some threshold value, otherwise deforming in a finite way like solids. According to the EN 3219, the threshold value where the liquid-solid transition occurs is a material's yield point.

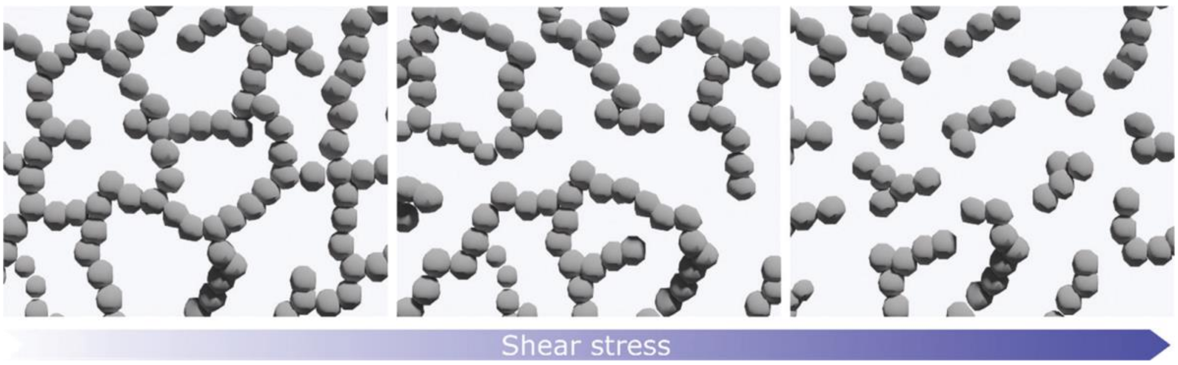

Figure 22. Shear thinning behaviour of a material under shear stress (Tagliaferri et al. 2021 p. 544).

Figure 22 illustrates shear thinning behaviour. Shear stress being above the material's yield point the microstructure brakes down and the material turns flowable and printable.

A material’s yield point can be evaluated with different flow curve fitting methods and viscosity using a rotational viscometer with a defined shear rate (EN 3219), (Tagliaferri et al. 2021 p. 544-546). Rheological tests simulate applications where a stress is needed to extrude the material through a small nozzle or an orifice. Some shear thinning materials may have two different yield stress values: Static yield stress, which is the stress required to flow from a rest state, and dynamic yield stress, which is the minimum stress required for a fluid in motion to continue flowing. For a shear thinning material to flow through the nozzle, it must overcome dynamic yield stress, whereas sufficient static yield stress is required to resist deformation after dispensing (M’Barki et al. 2017 p. 5). Figure 23 illustrates the rheological response of an ideal printable material.

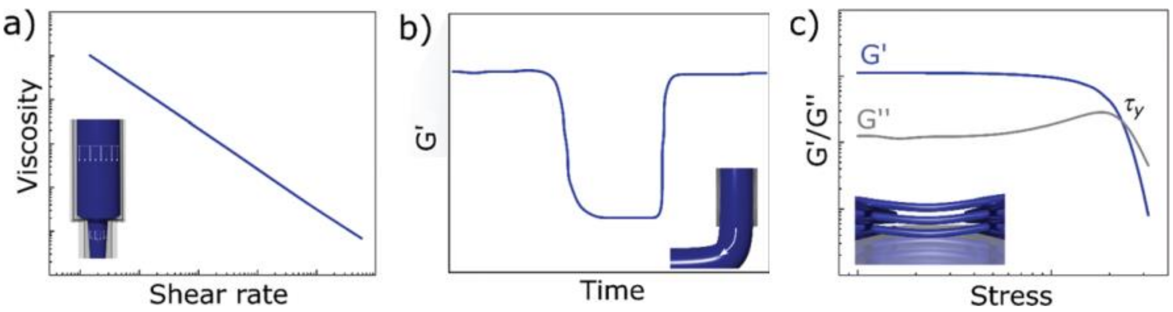

Figure 23. The rheological response of a printable material (Modified from Tagliaferri et al. 2021 p.545).

Figure 23 exemplifies an ideal rheological response of well printable ink. A desired shear thinning behaviour of material where the material’s viscosity decreases under shear rate (a). Elastic G′ and viscous G″ moduli parameters represent how elastic and viscous the ink is. During material extrusion (b) it is required that the viscous moduli G″ is greater than the elastic moduli G′ for the ink to flow. Instant liquid-solid transition mimics material structural regeneration at rest after extrusion (b). Sufficient elastic moduli G′ retains the printed characteristics (c) and in conjunction with a rapid liquid-solid transition improves accuracy. (Tagliaferri et al. 2021, Pp.543-546)

Guideline values for G′ and G″ can be found from literature for ink formulation. In general, both the G″/ G′ ratio and the G′ - G″ difference should be considered together. As a summary: Sufficient elastic moduli G′ is needed for structural strength. G′ should be at least 200 Pa greater than the material's yield stress for rapid liquid-solid transition, which contributes to improving accuracy and minimal scattering. Also, G″/ G′ ratio less than 0.8 ensures rapid liquid-solid transition. The lower the ratio, the greater the ability to retain shape after ink deposition. (Casanova-Batlle E et al. 2021 p.3) (Tagliaferri et al. 2021 p. 543)

Rheological material properties have a direct connection to the additive manufacturing process parameters. Hereafter are some useful formulas that can be used to estimate material performance in relation to printability.

The empirical Herschel–Bulkley model is used to describe the flow behaviour of the shear thinning DIW material having flow index n <1 (Tagliaferri et al. 2021 p. 544), as equation 1 shows:

$$\tau = \tau_y + K\dot{\gamma}^n \tag{1}$$

where τ is a shear stress, K is the viscosity parameter and τ_y the yield stress. This expression can also be used for shear thickening behaviour, where the value of n is greater than 1.

Volumetric flow rate $\dot{Q}$ through a nozzle with a radius r and printing speed S is, as equation 2 shows:

$$\dot{Q} = Sr^2 \tag{2}$$

and since non-Newtonian viscosity depends on shear rate $\dot{\gamma}$, nozzle radius and material volumetric flow rate have the following dependency with it, as equation 3 shows: (M'Barki et al. 2017 p.5)

$$\dot{\gamma}_{max} = \frac{4\dot{Q}}{\pi r^3} \tag{3}$$

The dependency above is useful for determining a non-Newtonian material's behaviour in relation to the nozzle diameter and printing rate. Some fluids will benefit from high shear, while for others it might be critical to maintain a low shear mode. It is noteworthy to stress that highly filled dispersions and polymer particle pastes without enough plasticizer typically display shear thickening behaviour (Anton Paar 2021). If the material behaviour is such and nozzle clogging occurs, the parameters above must be adjusted to lower the shear rate.

After the material has been successfully extruded out of the nozzle it should rapidly develop a high enough yield strength to resist deformation. In an optimal DIW process wise situation, the recovery of the ink's elastic properties should happen relatively quickly after deposition to avoid the collapse of the structure and to improve shape accuracy. The material recovery and its ability to maintain shape in relation to material properties can be estimated with relatively simple means.

M'Barki et al. (2017) introduced a formula to find the minimum yield stress σ_y^{dyn} necessary to support a printed structure's own weight and to avoid slumping under the gravity and capillary forces, as equation 4 shows:

$$\sigma_y^{dyn} \geq \gamma R^{n-1} + \rho g h \tag{4}$$

where γ is the suspension surface tension, R the nozzle diameter and ρgh the gravitational force (Tagliaferri et al. 2021 p.545) (M'Barki et al. 2017 p.7) At M'Barki et al. paper, the surface tension of a yield stress fluid is discussed more in detail.

The elastic G′ moduli defines the ability of a structure to be unsupported. Smay et al. (2002) formulated, that when limiting the maximum acceptable deflection equal to 5% of the nozzle or filament diameter D the expression for minimum elastic moduli is, as equation 5 shows:

$$\mathrm{G}' = 1.4\gamma \left(\frac{L}{D}\right)^4 D \tag{5}$$

where γ is the specific weight of the ink and L is the length of the spanning filament (Lewis J. 2002 p.248) (Tagliaferri et al. 2021 p.545).

2.4.2 Print parameter optimization

Additive manufacturing in general is highly affected by various process parameters. The selection of correct process parameters is the key for successful printing (Mohamed O. et al. C. et al. 2014 p.43), therefore several methods and strategies have been utilized to improve the quality of AM parts (Table 2) Adapting these optimization methods for additive manufacturing of novel materials, without prior information on the correct printing parameters and material behaviour is found to be difficult. Therefore, the search for the correct AM parameter combinations is still largely determined by trial and error (Abdollahi et al. 2018 p.2). Abdollahi et al. (2018) introduced a more systematic approach to find optimal printing parameters. Based on their method, expert judgement was used to select selecting relevant printing factors and decision making algorithms to search for print parameter combinations. Statistical software used in industrial process control such as the Minitab program, may be useful for uncovering hidden relationships between printing variables (Minitab).

Table 2. Comparison between the common experimental designs and optimization techniques (Mohamed O. et al. C. et al. 2014 p.50)

Capability	Techniques							
	Taguchi method	GA	Fuzzy logic	Gray relational	ANN	GMDH	Factorial design	RSM
Understanding	Normal	Difficult	Difficult	Normal	Moderate	Moderate	Easy	Moderate
Multi-response optimization	No	Yes	Yes	Yes	Yes	Yes	No	Yes
Uses	Widely	Rarely	Rarely	Widely	Widely	Rarely	Widely	Widely
Shape of the experimental region	Regular or irregular	Regular or irregular	Regular or irregular	Regular or irregular	Regular or irregular	Regular or irregular	Regular only	Regular only
Computational time	Short	Very long	Very long	Short	Long	Medium	Short	Short
Prediction accuracy	Low	High	High	Normal	Very high	High	Normal	Very high
Models linear dynamics	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
Models non-linear dynamics	No	Yes	Yes	No	Yes	Yes	No	Yes
Developing of mathematical model	No	No	Yes	No	Yes	Yes	Yes	Yes
Data requirement for a given output	Mid	High	High	Mid	High	High	Mid	Low
Optimal solution	Straight	Straight	Through model	Straight	Through model	Through model	Straight	Through model
Ability to study interaction effects between variables	Yes	No	No	Yes	No	No	Yes	Yes
Availability in simulation software	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes

Table 2 shows methods used for optimizing MEX additive manufacturing process parameters. The Taguchi method offers a simple and effective approach and can reduce the number of trials. Respectively, an artificial neural network (ANN) has an ability to identify complex and unknown print parameter and part quality relationships but requires training data. Prediction methods are not considered to be suitable for additive manufacturing (Mohamed O. et al. 2014 Pp.43-50).

Correct extrusion rate is a premise in material extrusion based additive manufacturing processes. The survey of printer parameters for a novel material starts form determining the extrusion rate range for consistent material extrusion (Figure 24) (Allevi 2020). Extrusion rate refers to the parameter in G code that controls material feed rate. Extrusion rate is also referred to as the k-value, E-axis or extrusion multiplier. It is worth to stress that printing speed and printing rate are mixed in literature. Printing rate is the measure of manufactured material over a given time. Depending on the AM process, the printing rate is expressed in kg, mm or cm^3 / hr. Printing speed is the velocity of print head movement in mm/s.

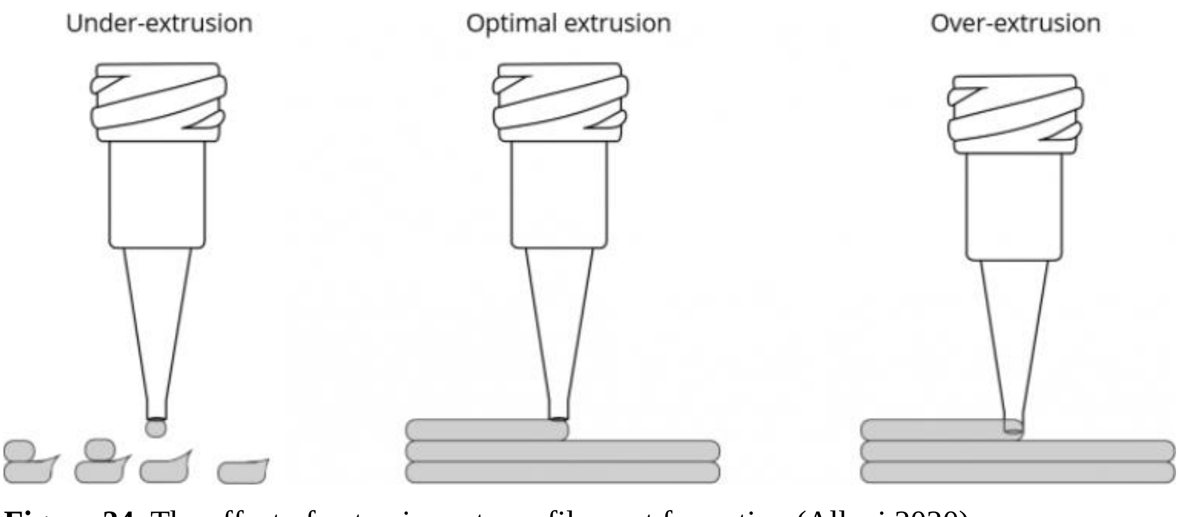

Figure 24. The effect of extrusion rate on filament formation (Allevi 2020).

Figure 24 shows an effect of extrusion rate on filament formation. Under-extrusion leads to an uneven filament and over-extrusion to inaccurate results (Allevi 2020). An extrusion test gives a parameter window for an achievable material extrusion rate in conjunction with a nozzle size and geometry, presented in equations 1, 2 and 3, respectively. The reason for under-extrusion may be nozzle clogging caused by material shear thickening behaviour or uneven material feed due to the lag of material feed.

Further testing is required to determine a material’s ability to form actual shapes. This is evaluated with various test geometries, starting with the simplest features possible (Figure 25).

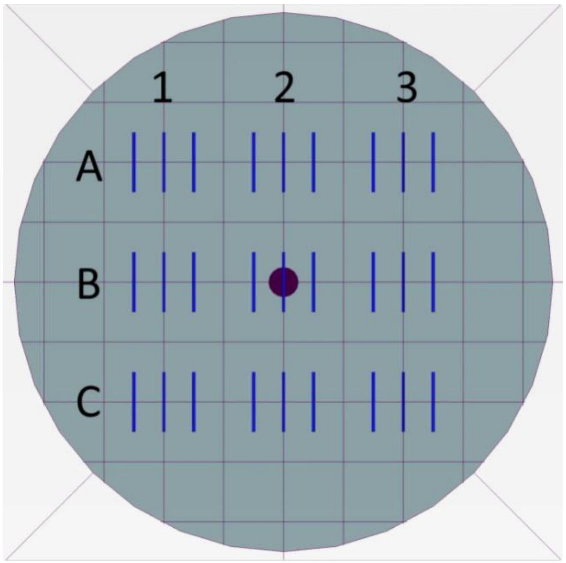

Figure 25. A single filament line test matrix including varying printing speeds (1,2,3) versus varying layer heights (A,B,C) (Allevi 2020).

Figure 25 shows a single line test matrix. The purpose of a single line test is to determine a print parameter window for proper filament deposition. The test is performed by printing individual filaments with different speeds and layer heights. The result is a line resolution map for the used pressure and nozzle. In figure 27 the numbers (1,2,3) refer to the tested printing speeds in relation to the varying layer heights (A,B,C) that remain the same across the row (Allevi 2020).

The search for correct printing parameters is a broad topic. It is not appropriate to address it in this context at full scale. A lot of research material is available especially for the MEX process which may be applicable.

3 DESIGN FOR ADDITIVE MANUFACTURING CASE STYDY

A blast wave is the principal attribute of an energetic material's ability to produce mechanical work, which is achieved by expanding product gases from the reaction. Undoubtedly, with conventional EM applications, a lot of energy is lost due to the absence of opportunity to direct the pressure effect precisely. The current charge geometry based methods of controlling and directing the pressure effect have been through the effect of aspect ratio, shape, and location of an initiation point. Traditionally manufactured energetic material applications are confined to basic geometries, and the possibility of creating varying porosity, which can also be applied to the pressure energy direction altering, is limited (Ares 2021).

The utilization of additive manufacturing on energetic materials is still under development and no commercial application was found during literature search. The potential utilization of additive manufacturing for the construction of energetic materials offers several possibilities (Ares 2021), notably through a more flexible design. The ability to fabricate an arbitrary complex shape particularly designed for an optimal blast energy distribution in priority, is clearly a value adding additive manufacturing opportunity.

A pre-set additive manufacturing method for this thesis was MEX-DIV. The limitation of available resources and references regarding DIV, is that the focus has been on the ink's properties, formulation design, machine design, and on the printing parameter optimization but none have particularly focused on the product design from an additive manufacturing perspective. The objective of this thesis is to increase knowledge on this field and to provide some useful information for future research.

The DfAM design process is structured into three global stages (Chapter 2.2.2). For clarity, this chapter follows the same structure.

3.1 Additive manufacturing suitability exploration

In practice, the first stage in design for additive manufacturing enclosures a decision making process wherein different additive manufacturing processes and value adding opportunities are evaluated in respect to product requirements. In ISO-ASTM 52910 p.11: "if a part can be fabricated economically using a conventional manufacturing process and can meet requirements, then it is not likely to be a good candidate for AM". This is probably the case if the intention is to directly replace the mass produced bulk EM product as is. On the other hand, reasoning can be the lead-time to justify the use of additive manufacturing.

Usually, cost is the primary decision criterion and an obstacle for the utilization of additive manufacturing. Regarding EM applications, cost might not be the most critical factor. The definition of return of investment for energetic materials is not so straightforward. The production of highly specialised energetic materials for specific scenarios offers cost savings (Ares 2021). Aspects such as, reduction in supply chain complexity, on demand field manufacturing, performance and improved efficiency through material savings should also be considered on decision making.

The capabilities of additive manufacturing: Shape, hierarchical, material and functional complexity meet the performance considerations of energetic material well. EM products were found to be shape, density and porosity sensitive. A spherical shell concept is presented to realize an additive manufacturing shape and hierarchical opportunities and to demonstrate the DfAM methodology for a previously unobtainable EM geometry.

In addition to being a previously unobtainable geometry, the spherical shell is an interesting geometry for the propagation of a detonation wave. The hypothesis is that a shock wave produced at one pole of a spherical shell, converges at the opposite pole. The propagation of the shock wave in a reactive medium is determined by the released energy in the reaction zone providing amplification and support to the forward propagating shock wave. The shock wave propagates to the direction of where it gets its energy from, resulting in a different pressure distribution diffused into the surrounding. A spherical shell is a shape that cannot be manufactured with current EM manufacturing techniques.

The sensitivity of HE materials is affected by defects such as voids, cracks, and internal boundaries. (Rai N. & Udaykumar H. 2019, p.1) The hypothesis is that a lattice structure (Figure 27 a) has an influence on this sensitivity and can thus be utilized to control a HE material’s response to shock loading.

3.2 Product (re)design for additive suitability goals

Additive manufacturing is based on the 3D geometry description of a real part which is translated into build instructions for the AM machine. Besides the AM machine’s capabilities and material rheology, 3D model, file conversion, slicing and tool path design are crucial factors that can achieve an optimized part. Before proceeding with manufacturing, the 3D geometry description of the real part must be constructed (Figure 26).

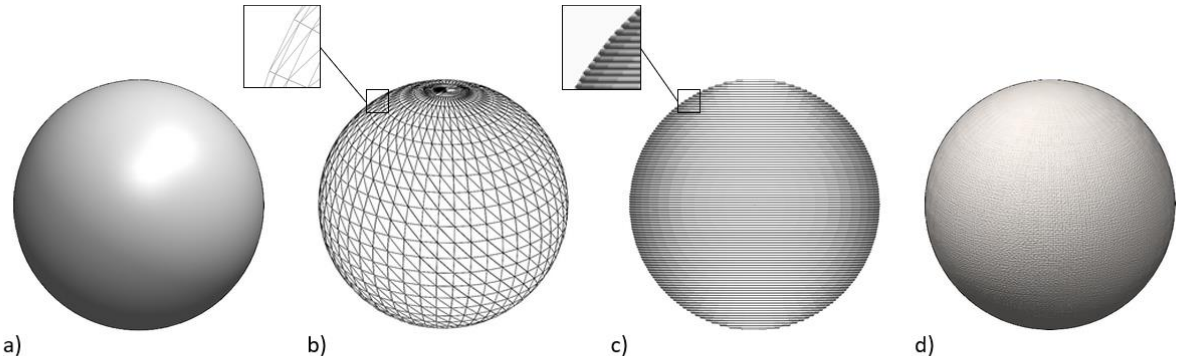

Figure 26. Additive manufacturing steps showing a) 3D geometry description, b) STL standard data interface, d) slicing and tool path design, and d) final part.

Figure 26 illustrates the simplified steps before proceeding with manufacturing (d). The part is designed in modelling software to create a 3D geometry model (a). The 3D geometry is converted into an STL (STereoLithography) file format (b) and sliced to get tool paths in the slicer program (c).

DfAM design methods are implemented into the 3D geometry in the design phase (Figure 26 a, Figure 27), often with parametric computer-aided design (CAD) software or more sophisticated engineering software especially intended for generative design and advanced manufacturing (ntopology 2021). Topology optimization and generative design DfAM tools were not required for the design. This was because the presented geometry is relatively simple and optimization in terms of the cost, material usage and build time objectives were considered not to be important. In addition, TO and GD produced organic shapes are not a suitable starting point for a novel material.

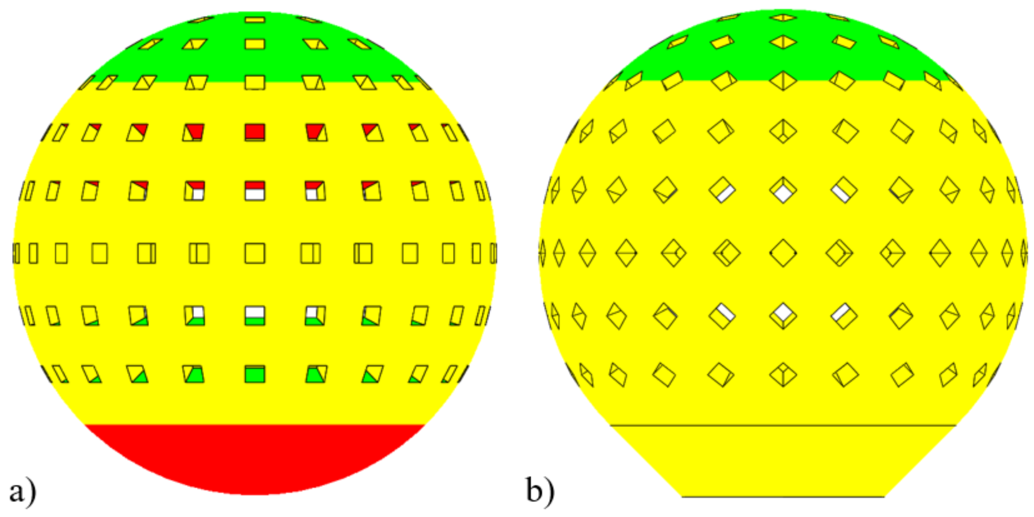

Figure 27. The application of DfAM design methods into the product design. a) initial design, b) adjusted design.

Figure 27 exemplifies a strategy of adjusting part design to make it more suitable to manufacture with additive manufacturing. In figure, a) presents the initial design. The desired part is a hollow spherical shape with holes conformally populated over the shell shape.

The part was first draft analysed in the CAD program to determinate overhanging areas where support material is required. Contact being too small between the deposited filament and the previous layer, support structures are needed. Avoiding supports is an inseparable part of design for additive manufacturing. The printing of supports increases build time, material usage and requires post processing. Ultimately, the need for support is reflected on the cost of parts. Considering the requirements of additive manufacturing method in the design phase, the need of support structures can be reduced.

The general guideline for overhang features in MEX additive manufacturing is 45° (3D HUBS 2021b) (Figure 28) which in most cases ensures that the features will be printed correctly. The guideline value for overhang is not generally applicable and varies depending on filament width and the layer height.

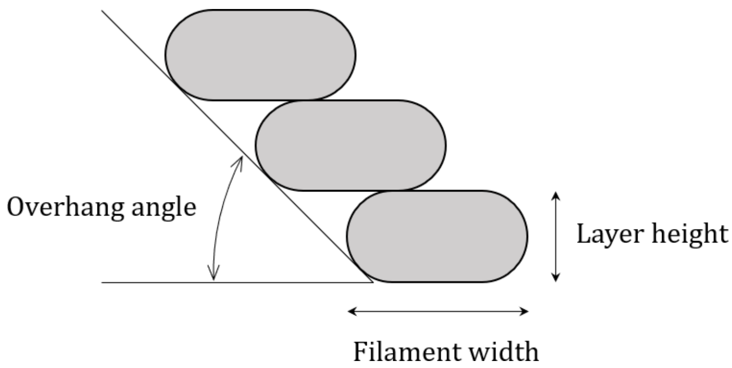

Figure 28. Definition of overhang angle

Figure 28 shows a general 45° overhang guideline angle. The overhang angle α can be estimated and has the following dependency in relation to filament width d and layer height h, as equation 6 shows:

.

$$\alpha = \tan^{-1} \frac{d*(1-f)}{h} \tag{6}$$

where the parameter f is a percentage overlap of the printout outlines. The suggested default is 33% (Omni3d. 2021). Information of the appropriate overhang value is needed at the design stage and should be experimentally verified with test geometries for novel materials. In practise, printing with a too small overhang angle means printing on air, respectively, an unnecessary use of support material should be avoided. For prototyping purposes in this case, the 45° value was successfully used.

In the prototype part (figure 27 a), the red colour indicates a region where the overhang angle is under the applied 45° limit value and support material is required. According to the analysis, support material would be needed for some holes and the larger region under. The materials elastic moduli G′ defines the structure's ability to be unsupported. Presented in equations 4 and 5, respectively.

The adjusted design is presented in figure 27 b. For holes, the need for support material can be avoided completely by rotating the unit cell 45 degrees. Since the unit cell is conformally populated over the shell shape, the change is repeated all over the pattern. During the MEX printing process, the underlying layers must be stable and connected to the printer build platform. The base of the part (Figure 27 b) was modified into a flat conical shape to obtain contact surface with the build platform and to remove the need for support material.

3.3 Geometry optimization to enable the product realization chain

The stage comprises of activities that aim to define the additive manufacturing process. The input for the manufacturing planning stage is a transfer 3D geometry description of the part, which is generated from the CAD design (Figure 29). Additive manufacturing uses an STL file format as a standard data interface. (Stratasys 2021)

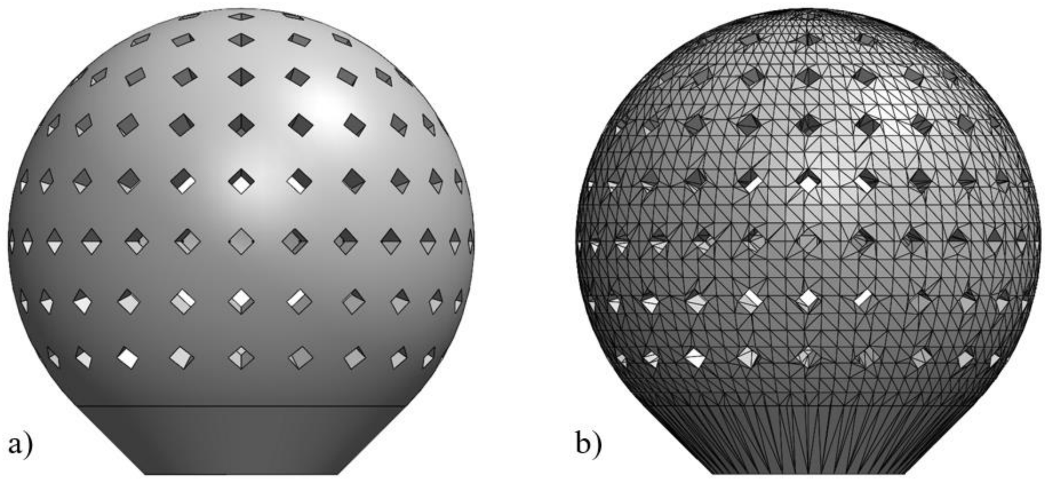

Figure 29. The effect of STL geometry approximation on 3D geometry.

Figure 29 illustrates the difference between native, CAD designed (a) and STL transfer file format 3D geometry description (b). The reason for the file format conversion between the CAD and slicer programs is that different CAD programs have their own unique file formats, and the capabilities to read and write file formats across the programs is limited. STL is the most popular and widely used format in additive manufacturing. (Stratasys 2021) STL is a triangulated representation of a 3D geometry, it describes the 3D geometry by approximating and splitting entire surfaces (a) into facets (b). The accuracy of the surface approximation has a direct link to the print quality. If the STL conversion is done coarsely the physical 3D printed part will be coarse and faceted as well. A more accurate triangulation increases the number of facets and file size which in turn unnecessary slows down the slicing. Finding a balance between triangulation accuracy and printing resolution is advised. It makes no sense to have more details in the STL file than the printer's resolution.

In addition to STL file conversion, slicing and tool path design are crucial factors that affect part quality. Slicing software is a tool for filament deposition route planning and layer design; it cannot fix poor part design. In the end, how efficiently the part can be built is determined at the design phase. A very important DfAM guideline is the consideration of printing orientation (Figure 30) already at the design stage, not only to avoid support material but also to improve part properties.

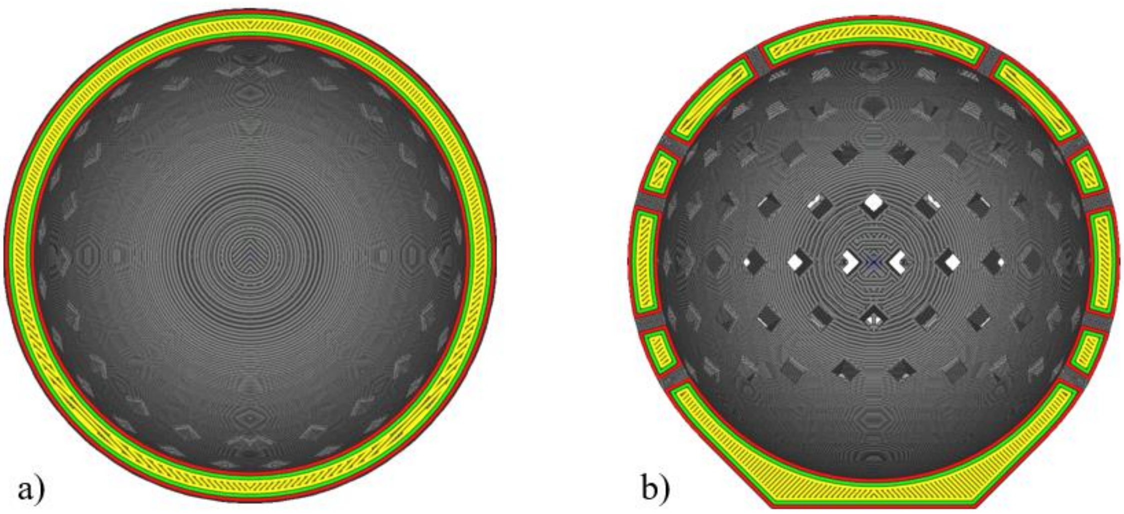

Figure 30. The effect of build orientation on filament construction.

Figure 30 illustrates a single layer of the part in different build orientations, viewing direction towards the build platform. Case a) can considered to be correct for the standard MEX process. The general way a slicer program constructs a filament deposition G-code instruction is illustrated with colours in the figure. Gray represents an underlaying build part, red and green wall filaments and yellow infill.

4 RESULT AND DISCUSSION

The main motivation for this thesis was to reconcile the potential of additive manufacturing with a novel energetic material application area. The hypothesis was, that by utilizing DfAM, value adding opportunities can be identified and the product can be optimized for additive manufacturing.

The DfAM process was demonstrated with three global AM design stages, which can be summarized and presented in a simpler form:

1) **System design.** Focuses on component specific requirements and defines whether AM is a suitable manufacturing method.
2) **Part design.** Contains modification of the original or a new design to suit the additive manufacturing technique.
3) **Process design.** Comprises additive manufacturing process planning, includes definition for e.g., part orientation, slicing scheme, support generation, printer parameter optimization and post processing.

The shape and hierarchical complexity capabilities of additive manufacturing were found to align with the performance considerations of energetic materials. EM products were found to be shape, density and porosity sensitive. The AM capabilities were implemented into the prototype design.

In the case of the presented prototype part, the DfAM methods were implement into the completely new fresh design. The presented design (Figure 32) is relatively simple and no advanced AM engineering software was needed. The prototype part was designed according to the DfAM guidelines to avoid support material completely and was successfully additive manufactured.

Figure 31. Printed prototype part designed according to the best practises of DfAM

Figure 32 shows a hollow spherical shape with holes conformally populated over the shell shape. All holes have an individual orientation in space. For a traditional manufacturing method such as casting, this kind of arrangement would require a mold opening in multiple directions. The forming of a hollow shape is virtually impossible for current energetic material manufacturing techniques.

Even though the infill was set to 100% in the slicer program, small gaps can be seen between the filaments. Due to the manufacturing method, material extrusion based AM processes exhibit some level of natural meso scale porosity, meaning small voids between the printed filaments (Figure 31). These voids cause uneven material distribution and structural anisotropy. (Rankouhi B. et al. 2016 p.477)

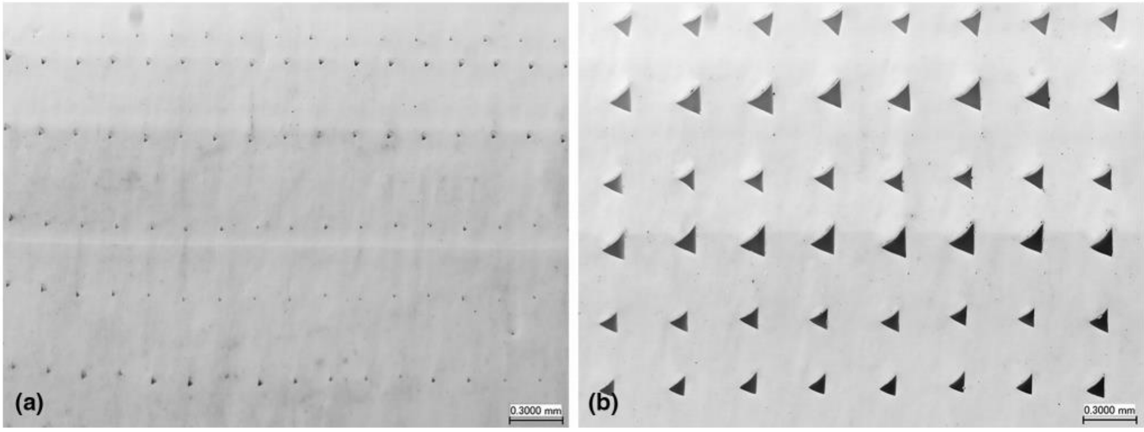

Figure 32. Mesostructure voids with (a) 0.2 mm and (b) 0.4 mm layer thickness. (Rankouhi B. et al. 2016 p.477)

Figure 31 shows void cavities between the filaments. In addition to the build orientation, the void pattern is based on filament deposition G-code instructions and can be therefore altered. It is generally well known how void patterns influence filament adhesion and mechanical response of the MEX-FDM parts, the parts are weaker and rapture more easily in the build direction. In the case of additive manufacturing processes where build orientation affects part performance, determining the build orientation in relation to the part performance requirements is important.

The formation of natural meso scale porosity can be seen as an opportunity for additive manufactured energetic materials. The sensitivity of HE materials is affected by defects such as voids, cracks, and internal boundaries. In addition, experiments have shown that shock energy can be altered by converging shock waves.

6 CONCLUSION

The additive manufacturing shape complexity capability, which further permits shape optimization, can facilitate energetic compositions with previously unobtainable geometries. The effect of shape on the dynamics of the generated pressure wave is already utilized on EM products. DfAM offers a variety of tools for shape optimization (TO,GD,CFD). The usefulness of the current tools is questionable regarding EM products. The Existing application of topology optimization for additive manufacturing has been to reduce the cost of parts through material use and build time, in respect to optimal strength. Mechanical strength is not an issue for EM products. Available topology optimization tools do not offer a solution in respect to the optimal distribution of a blast wave. A baseline analysis of the shape effect is available, for now engineering must be done through knowledge based engineering (KBE). Presumably with a topology optimization algorithm capable of constructing a shape based on the desired blast wave profile, products could be designed to be more efficient.

The effect of voids in additive manufactured energetic material products remained unresolved, no research data was found. The effect of voids, and control over micro or meso scale porosity through additive manufacturing could be a right direction for future research.

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