CHEMICAL ENGINEERING TRANSACTIONS
VOL. 103, 2023

A publication of
AIDIC
The Italian Association
of Chemical Engineering
Online at www.cetjournal.it

Guest Editors: Petar S. Varbanov, Panos Seferlis, Yee Van Fan, Athanasios Papadopoulos

ISBN 979-12-81206-02-1; **ISSN** 2283-9216

DOI: 10.3303/CET23103079

Structural Topology Optimization of Metal Hydride Gyroid Container for Hydrogen Storage

Luthfan Adhy Lesmana[a], Muhammad Aziz[b,*]

[a]Department of Mechanical Engineering, The University of Tokyo, 7-3-1 Hongo,Bunkyo-ku, Tokyo 113-8656, Japan
[b]Institute of Industrial Science, The University of Tokyo, 4-6-1 Komaba, Meguro-ku, Tokyo 153-8505, Japan
maziz@iis.u-tokyo.ac.jp

Many engineering applications can benefit from reducing the weight of structures. While approaches for optimizing the topology of both continuous solids and discrete frame structures have been available for some time, the introduction of additive manufacturing procedures has made it possible to create more complex geometries. On the other hand, one of the greatest challenges in using hydrogen fuels lies in the development of hydrogen storage systems. Among hydrogen storage technologies, the storage of hydrogen in solid-state compounds like Metal Hydrides (MH) appears to be the most feasible solution, as it is safer and has a higher hydrogen volumetric density. However, one downside of MH is its gravimetric density, which prevents its effective use in mobility applications. A novel approach to solving this problem is to integrate the reactor tank into the frame and chassis of the vehicle itself. In this study, a topology-optimized MH container based on a gyroid structure is proposed. The topology optimization method is adopted for the vehicle part geometry that is already filled with the gyroid structure. The proposed geometry is then analyzed with Finite Element Analysis (FEA) and Computational Fluid Dynamics (CFD) to assess its mechanical and heat transfer characteristics, as well as the hydrogen charging rate capability of MH inside the structure. The use of topology optimization with the SIMP method resulted in a 17 % increase in overall chamber volume and almost 50 % reduction of HE material, which affected the overall volumetric and gravimetric density of the reactor. Although the strength of the optimized structure showed a measurable decline, it was able to withstand the given mechanical shear load. The displacement of the structure showed more than usable rigidity of less than 0.2 mm displacement, making it suitable for use in assembly parts like vehicle frames or chassis. The optimized structure also showed a slight increase in charging rate, making it a promising approach for designing the container.

1. Introduction

Energy utilities play a crucial role in shifting towards sustainable energy sources, contributing to energy security and reducing carbon emissions. Investors prioritize firms dedicated to climate preservation, and as a result, energy utilities are transitioning towards cleaner, more sustainable, and affordable energy while setting ambitious goals for reducing CO_2 emissions. Hydrogen is a promising alternative energy carrier with reduced greenhouse gas emissions and diverse primary sources, making it an attractive option for next-generation automobiles and stationary sectors. However, challenges such as efficient hydrogen storage, green hydrogen generation, low-cost distribution, and cheaper, more durable fuel cells hinder its widespread adoption. Hydrogen storage is particularly challenging due to its low volumetric energy density compared to other gases. Achievable targets set by the US Department of Energy include a gravimetric capacity of 5.5 wt.% and a volumetric capacity of 40 $g \cdot L^{-1}$ at an operating temperature range of -40 to 60 °C and under a maximum delivery pressure of 12 bar. (Murray et al., 2009).

Although metal hydride (MH) is considered an excellent candidate for stationary hydrogen storage, there are concerns about its use in the mobility sector due to its low gravimetric hydrogen density.MH is formed by a metal compound that experiences the sorption of hydrogen. The pressure-composition-temperature (PCT) relation curve can be used to explain this phenomenon. An initial solid solution of metal (α phase) is formed just before the hydrogen pressure and concentration start to increase. MH formation (β phase) starts to form under these

Paper Received: 07 June 2023; Revised: 02 August 2023; Accepted: 26 August 2023
Please cite this article as: Lesmana L.A., Aziz M., 2023, Structural Topology Optimization of Metal Hydride Gyroid Container for Hydrogen Storage, Chemical Engineering Transactions, 103, 469-474 DOI:10.3303/CET23103079

conditions, and once α and β phases are in equilibrium, the curve forms a plateau. This reaction can be expressed as Eq(1).

$$M + \frac{x}{2}H_2 \leftrightarrow MH_x + Heat \tag{1}$$

MH technology offers promising hydrogen storage capabilities due to its high hydrogen density per unit volume and safe operational conditions. However, its usage in mobile applications is restricted due to its low hydrogen density per unit mass and slow charging and discharging rates. To overcome this limitation, one possible approach is to miniaturize and lighten MH reactors and incorporate them into the building components of mobile applications, like the integration of lithium batteries into electric vehicles.

In contrast, open-cell porous structures, particularly TPMS structures, have been extensively investigated for their potential application in developing bone implants and scaffolds (Dong and Zhao, 2021). The shape of the TPMS is defined by equations that describe the location of a surface, enabling the investigation of different mathematical functions to enhance mechanical properties while retaining a high level of porosity. TPMS structures possess good permeability, which promotes bone growth and remodeling. Compared to other lattice structures based on a grid, TPMS structures, particularly the gyroid, have been observed to exhibit lower levels of stress concentration under compression load (Lu et al., 2022).

TPMS can be created by utilizing mathematically restricted cell shapes that are arranged asymmetrically in 3D space. These geometries are characterized by two interlaced networks of spaces, which possess a zero-mean curvature. As a result, they have been extensively studied for their potential application in heat exchangers, where they have been proven to enhance turbulence and improve heat transfer performance (Lord and Mackay, 2003). TPMS has been catalogized with various forms, including Schwartz-p and Schoen Gyroid, with each of them can be described from the equation as follows.

Schwarz P

$$cos(x) + cos(y) + cos(z) = C \tag{2}$$

Schoen Gyroid

$$cos(x).* sin(y) + cos(y).* sin(z) + cos(z).* sin(x) = C \tag{3}$$

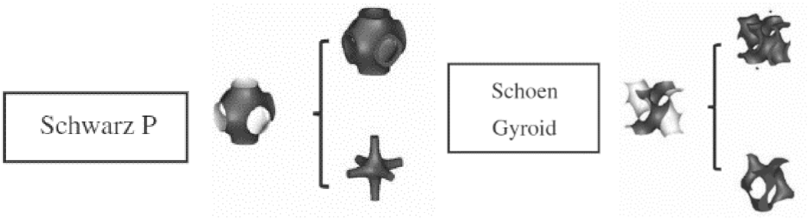

Figure 1: Visualization of Schwarz P and Schoen Gyroid (Thomas et al., 2018)

The spaces mentioned earlier can be differentiated into sheet and skeletal regions, as depicted in Figure 1. The Cartesian coordinate system is represented by x, y, and z, with the constant C representing porosity.

The author`s previous study has previously utilized TPMS as an MH reactor and observed improved heat transfer and hydrogen absorption and desorption rates. However, the proposed design resulted in a high volume density penalty as only 30 % of the overall volume could be used for the MH chamber (Lesmana and Aziz, 2023). One way to reduce volume is to optimize the topology.

In this study, a topology-optimized MH container based on a gyroid structure is proposed, and the topology optimization method is adopted for the vehicle part geometry that is already filled with the gyroid structure. Topology Optimization (TO) is a design strategy that aims to find the best material distribution in each design space while meeting a set of constraints and fulfilling a set of objectives (Wu et al., 2021). In this method, the design space is partitioned into finite elements, and the qualities of each element are modified to meet the desired optimization goal. The Solid Isotropic Material with Penalization (SIMP) method is considered convenient for numerical implementation. The use of a TPMS-based heat exchanger as a metal hydride hydrogen storage reactor has also been explored. These novel approaches aim to address the limitations of current hydrogen storage methods and improve the efficiency and safety of hydrogen-powered vehicles.

2. Methods

The TO method used in this study aims to minimize the volume of the final gyroid structure while meeting stress and displacement constraints by optimizing the densities of the elements in a given design domain. This density optimization serves as a guide for where to reduce volume, as stated in Eq(4).

$$\begin{cases} \text{Find } \rho = (\rho_1 \rho_2 \cdots \rho_n)^T \\ \text{Min } V = \sum_{i=1}^{n} \rho_i v_i \\ \text{S.t.} \begin{cases} F = Ku \\ u \leq u' \\ \sigma \leq \sigma' \\ 0 \leq \rho_{min} \leq \rho_i \leq \rho_{max} \end{cases} \end{cases} \tag{4}$$

$$E_i = {\rho_i}^p E^0 \tag{5}$$

where ρ is the given design space, V is the gyroid solid volume, F is the load given, K is the global stiffness matrix, u and u' is the global displacement and the displacement constraint, σ is the von Mises stress vector, σ' is the stress constraint. The optimization objectives use the SIMP method (Wu et al., 2021) to define the density so that it can range from 0 to 1 while maintaining a minimum lower bound of $\rho_{min} = 0.001$ when calculating equilibrium. Additionally, a penalization power parameter (p) greater than 1 is introduced, in this research we use 3 as penalization power parameter to increase the resolution of generated TOed structure. Finally, the Young's modulus of each element is determined using Eq(5). E^0 is Young's modulus of the material in the solid state. The relationship of ρ and E has been studied where ρ=3 shows the preferable ratio of young modulus and relative density.

This study uses the simple case of a cantilever problem with a surface load of 1,000N on -z-direction on one face and fixed on the opposite face visualized in Figure 2. Figure 2 also visualizes the 5,030,023 cells that are used for the TO method and FEA analysis. Generated model of optimized structure utilized as scalar function datapoint where a TPMS gyroid structure then thickens the wall based on the density map. The heat exchanger design used wall thickness mapping results on gyroid with 10 mm cell size.

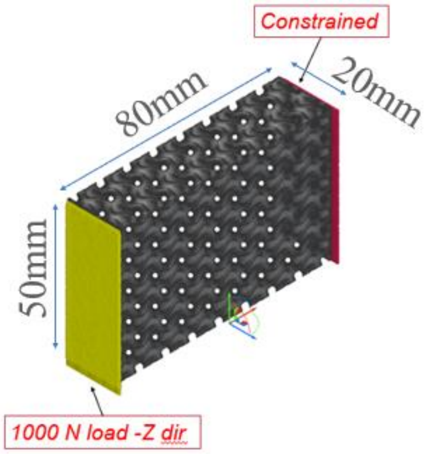

Figure 2: Dimension case study with load and constraint

Strength analysis of the optimized reactor is performed in an ANSYS software package, with boundary loads (1,000 N shear load) and fixed support applied, as shown in Figure 2. The same analysis boundary was utilized to validate the TO method and also find a reduction in the strength of the new optimized shape. The material properties of Al-Si10-Mg are utilized for both TO and FEA analysis, as it is the most frequently used material for metal additive manufacturing methods and is considered the only process capable of producing TPMS design, especially gyroid (Ishfaq et al., 2021). The Young modulus of the material is 64 GPa, and the yield stress is 256 MPa, extracted from the material manufacturer's specification.

3. Results and discussion

Figure 4 illustrates the geometry of the TO result, which has a scale factor of 0.5 and a front wall that thickens by 3 mm to ensure the structure can hold the given load. Despite the varying cases and loads, this structure shares similarities with the solid cantilever case from the previous work mentioned in the introduction. As stated in the method, this study strategy involves mapping the wall thickness based on the scalar function of the TO result. This variation in wall thickness can be observed in the final design that generated a trace of the TOed cantilever as the thicker wall and unused material as the thinner wall.

By analyzing the geometry of the reactor wall structure, we can identify chambers that are suitable for heat exchanger fluid and storing metal hydride by measuring their volume. Figure 4 shows a comparison of the volume of chambers in the TPMS gyroid with a 3 mm wall thickness and in TO TPMS gyroid structure. The optimized TPMS gyroid with 3 mm wall thickness achieves a 49% reduction in required material for the wall structure while increasing the chamber volume by around 17% with little difference between the two chambers. This geometrical improvement enhances the practicality of the reactor by allowing for more metal hydride material to be stored and increasing the volumetric energy storage density of the overall system. Reducing the wall heat exchanger (HE) material also results in a lighter structure, which improves its gravimetric density. Since the material is isomorphic, the result of reducing weight is proportional to the volume reduction (49%).

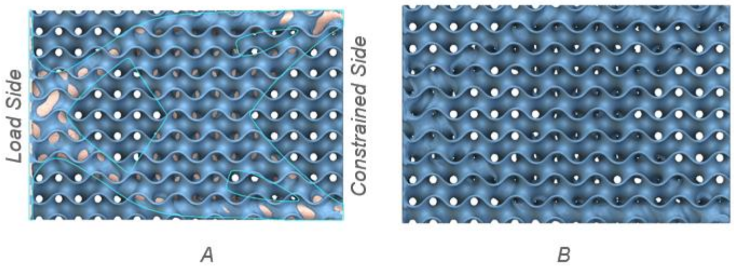

Figure 3: TO result adapted into wall thickness ranging from 1-3 mm (a) and gyroid structure after implementation of variable wall thickness (b)

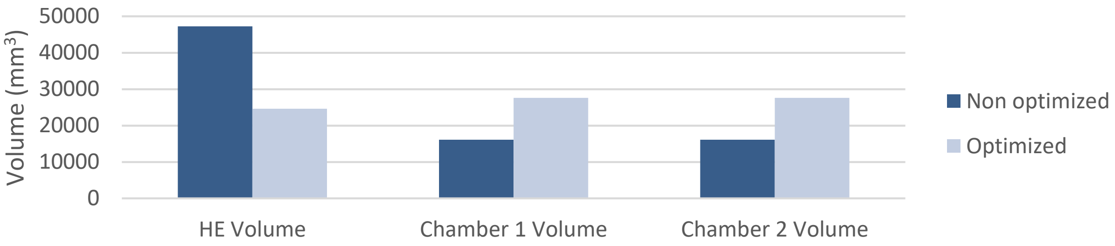

Figure 4: Volume (mm^3) comparison of optimized and non-optimized structure

Figure 5 visualizes the FEA analysis results that show both Von Misses distribution and material displacement under load. Maximum material displacement of 0.04 mm that resulted in the edge region of the unoptimized all 3 mm wall thickness structure observed. Maximum Von Misses concentration is observed nearby the constrained area on the unoptimized structure, with around 90 MPa of stress on the top side also observed. On the other hand, the optimized structure shows a higher displacement distance with 0.09 mm of displacement and around 127 MPa of maximum stress concentration observed nearby the constrained side on the bottom part. Although the amount of displacement and stress is different, Figure 5 shows a similar concentration map for both values. This result shows that the structure behaves the same mechanically, demonstrating the same area where the highest displacement and material stress concentration occurs with a different value. These results validate the purpose of optimizing the strategy deployed in this study, reducing material without altering the function of the structure.

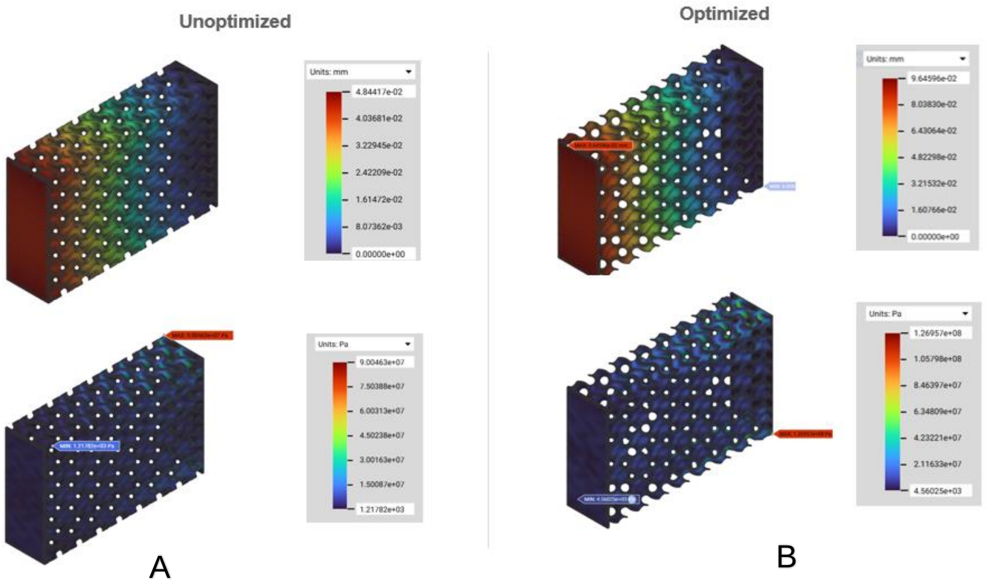

Figure 5: FEA study results with displacement (top) and Von Mises stress distribution (bottom) of unoptimized structure (a) and TOed structure (b)

Further analysis of the cut section of the structure visualizes the effect of optimization and strategic material removal as visualized in Figure 6. The strain or stress concentration on the unoptimized structure shows that the uniformly thick wall for the gyroid has low strain material that indicated by darker blue color. Unlike the unoptimized structure, the TOed structure shows thicker sections receive higher strain, and thinner structures receive less strain on average. In other TO cases, this darker area is usually removed to keep the structure lighter. But since the current case is for an MH reactor, more chamber volume per overall reactor volume is desired to make the MH volumetric density high. Keeping this structure will increase the hydrogen capacity while adding extra strength because of more structural material that keeps the reactor ridged and able to withstand more load.

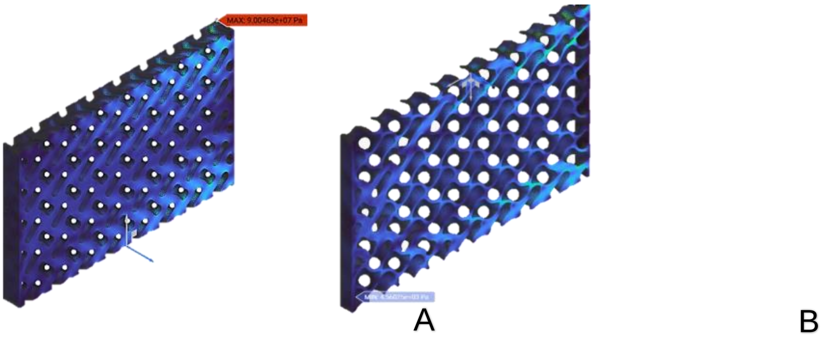

*Figure 6**:** Strain distribution on the cut section of the un-optimized (a) and TOed (b)*

The previous study of the author's works has developed a numerical model to simulate the charging rate of hydrogen on MH validated with existing experiment data (Singh et al., 2015). By using the same model, with the same mesh size and MH material properties, alongside the same ambient parameter and charging pressure as the previous study (Lesmana and Aziz, 2021), the charging rate of extracted chamber geometry from both unoptimized and optimized structures were simulated. The result is then visualized in Figure 7. The figure shows that although total hydrogen capacity per weight as fraction reach is the same, the optimized structure has a faster charging rate for the first 1,000 s. This faster charging rate up until 90 % of hydrogen capacity also means measurable more hydrogen absorbed at a given time, when considering optimized structure increases the MH chamber volume by 17 %.

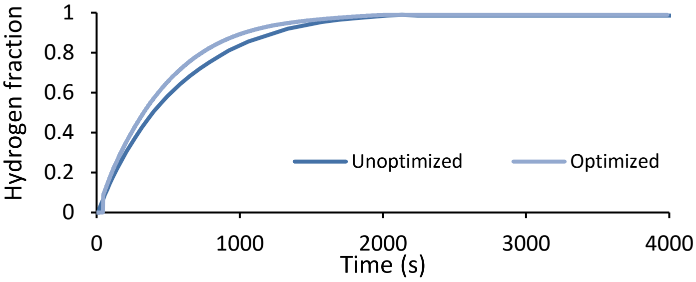

Figure 7: Hydrogen fraction of optimized and non-optimized structures.

4. Conclusion

TO of the reactor structure for MH has been investigated with its overall increase in capacity, strength, and hydrogen charging capability. By utilizing TO with the SIMP method, a 17 % increase in overall chamber volume and almost half reduction of HE material directly affect the overall volumetric and gravimetric density of the reactor. The strength of the optimized structure shows a measurable decline within the designed load based on the case determined during the TO method. However, the optimized structure proved able to withstand the given mechanical shear load. Displacement of the structure also shows more than usable rigidity since material breakage of the same material is around 9 % of the length of the overall structure or 0.9 mm. This rigidity under load also further increase its usability when utilized in assembly parts like vehicle frame or chassis. Typical assembly in the manufacturing process requires a certain amount of size tolerance so the assembly can work without failing or being locked to each other. Standard large fitting assembly uses 0.2 mm of tolerance, still more headroom in geometry for the optimized structure to work as an assembly part even under load. A slight increase in the charging rate also further proves the usability of the approach. By using TO to optimize MH TPMS gyroid structure as a novel approach for designing the reactor, the idea of a hydrogen-based car to use MH bed for hydrogen storage is already promising.

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