nature portfolio

Peer Review File

Free-form thermal cloaks in three dimensions

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This file contains all reviewer reports in order by version, followed by all author rebuttals in order by version.

Version 0:

Reviewer comments:

Reviewer #1

(Remarks to the Author)
This paper employs transformation theory and de-homogenization to investigate the design and practical application of a three-dimensional thermal cloaking system composed of three-dimensional lattice microstructures. Based on collected data on homogenized thermal conductivity, the authors optimize the size of the microstructures to achieve the desired anisotropic thermal conductivity and position them accordingly to design the overall structure. Because the entire structure is designed theoretically, full-scale simulations are not required, and the computational cost may appear low. However, in practice, the size of each microstructure is optimized for every spatial location, and when data collection for homogenized thermal conductivity is included, the computational cost increases accordingly. The obtained numerical results are impressive, and the resulting structure is intriguing. Nevertheless, given the claimed methodological advances and their apparent effectiveness, it remains unclear whether this paper meets the publication standards of Nature Communications (though this reviewer's overall impression is not negative). This reviewer will consider the authors' revisions and responses to the comments below before deciding whether to recommend publication.

[Comment 1] Is the main significance of this paper that it extends the authors' previous theory from their Nature Communications paper [10] to a three-dimensional system? Theoretical constructs such as de-homogenization, transformation thermotics, and the wave function expression are again employed in the present study, suggesting that theoretical progress may be limited.

[Comment 2] It is unclear what the widths b_1, b_2, and b_3 refer to. Please indicate these clearly in the figure showing the microstructure in the supplementary material.

[Comment 3] The characteristic size of the microstructure appears comparable to the macroscopic dimensions, which raises concerns about the validity of the scale separation assumption in the de-homogenization procedure. I recommend providing quantitative evidence or discussion to confirm that scale separation is satisfied. In addition, please identify and illustrate the Representative Volume Element (RVE) used in your analysis and clarify how it represents the overall microstructural behavior.

[Comment 4] Although the proposed method is claimed to outperform other thermal cloak design approaches, particularly topology optimization, the comparison presented in the introduction is not sufficiently comprehensive. Please include a more detailed comparison of the various methods available for designing thermal cloaks, discussing their respective advantages, limitations, and computational costs.

[Comment 5] Related to the above point, potential reviewers may wish to see how the computational cost of this approach compares with other methods (e.g., topology optimization). A fair comparison should include all relevant computational efforts, including preparatory steps such as the collection of homogenized thermal conductivity data.

[Comment 6] Thermal conductivity should be expressed in units of W/(m·K) rather than W/mK to make it clear that the kelvin unit is in the denominator.

[Comment 7] The paper's tone is sometimes overly laudatory, with phrases such as ``elegant and general transformation theory'' that obscure the main message. Unless these are technical terms, please revise such expressions throughout the manuscript to maintain a more neutral and objective tone.

Reviewer #2

(Remarks to the Author)
This manuscript realizes three-dimensional thermal cloaking with arbitrarily complex shapes via a 3D lattice composite. Numerical and experimental results both verify good thermal manipulation performances. Unfortunately, I do not recommend it for publication due to lacking novelty. The progress on realizing a 3D cloak with arbitrary 3D space is not interesting enough to publish in a journal like Nature Communications. Some specific concerns are listed below.
Page 1. I do not agree with the claim "Real-world applications are three-dimensional, and how to realize the elegant transformation theory in a general 3D domain and engineer free-form 3D omnidirectional thermal meta-devices remains far from being understood." Is transformation thermodynamics not understood in general 3D domain? There are a lot of works on that. Cloaks with complicated shapes were extensively studied in the field of electromagnetism and acoustics (1-7). They were later transferred to heat diffusion fields (8-10). Han et.al. and Liu et.al. designed arbitrarily polygonal cloaks with homogeneous and non-singular parameters (11-12). Xu et. al. designed arbitrary polygonal thermal schemes using the linear mapping functon(13-16).
1) Diatta, A. Nicolet, S. Guenneau, and F. Zolla, Opt. Express, 2009, 17, 13389.
2) Nicolet, F. Zolla, and S. Guenneau, Opt. Lett.,2008, 33, 1584-1586.
3) W. X. Jiang, J. Y. Chin, Z. Li, Q. Cheng, R. Liu, and T. J. Cui, Phys. Rev. E, 2008, 77, 066607.
4) H. Ma, S. Qu, Z. Xu, and J. Wang, Opt. Express, 2008, 16, 15449-154454.
5) M. Rahm, D. Roberts, J. Pendry, and D. Smith, Opt. Express, 2008, 16, 11555-11567.
6) G. Zhu, J. Appl. Phys., 2013, 113, 163103.
7) Q. Li and J. S. Vipperman,Appl. Phys. Lett., 2014, 105, 101906.
8) T. H. Li, D. L. Zhu, F. C. Mao, M. Huang, J. J. Yang, and S. B. Li, Front. Phys., 2016, 11, 110503.
9) Peralta and V. D. Fachinotti, Sci. Rep., 2017, 7, 1-8.
10) X. Wang, S. Qu, X. Wu, J. Wang, Z. Xu, and H. Ma, J. Phys. D: Appl. Phys., 2010, 43, 305501.
11) T.Han, C. Qiu, and X. Tang, J. Optics, 2010, 12, 095103.
12) Y.Liu, W. Guo, and T. Han, Int. J. Heat Mass Transfer, 2017, 115, 1-5
13) G. Xu, H. Zhang, and Y. Jin, Energ. Convers. Manage., 2018, 165, 253-262.
14) G. Xu, X. Zhou, and Z. Liu, Int. Commun. Heat Mass, 2019, 108, 104337.
15) Q. Li and J. S. Vipperman, J. Appl. Phys., 2018, 124, 035103.
16) Q. Ji, et al. ES Energy Environ., 2020, 7, 29-39
Besides, 2D omnidirectional thermal meta-devices has been studied. They are also mentioned by the authors, such as references [9] [11] [16] [22] [24]. Why to claim "engineer free-form 3D omnidirectional thermal meta-devices remains far from being understood"? What exactly is far from being understood? Is there any different principle or any paradigm shift when extending from 2D to 3D? To me, the 3D case is simply more complex, labor-cost and time consuming, while shows no fundamental difference with 2D case in the design principle.
Related with the first question, what is the main contribution of this work? Is it an incremental progress from 2D to 3D? what is the novel design principle or new avenue here? Without such highlighted novelty, the manuscript is not convincing to publish in Nature communications.
In Fig.1, the local microstructure and its effective conductivity have been well described in literature (Q. Ji, et al. ES Energy Environ., 2020, 7, 29-39) which is based on two-scale homogenization method. In their works the parameters of such structures were also optimized to design 3D thermal cloaks. In this manuscript the authors employ identical microstructures and similar design process, without citing this work and without showing any advantage over the published work.
I would raise the doubt on novel contribution again after reviewing the whole manuscript. The basic idea is to optimize the microstructure parameters so that they demonstrate the target anisotropic graded thermal conductivities. Then the ideal conductivity tensor required by the thermal device is replaced by the optimized microstructures. Is that correct? Unfortunately, this approach has been well depicted in previous works, though mainly on regular shapes and 2D. In this work, the homogenization method, the inverse design and optimization methods all did not show much novelty (International Journal of Heat and Mass Transfer 169, 120948; International Journal of Heat and Mass Transfer 196, 123149 (6)).

Reviewer #3

(Remarks to the Author)
This manuscript presents a full design-to-fabrication framework for omnidirectional three-dimensional thermal cloaks with free-form inner and outer boundaries. The authors integrate 3D de-homogenization with a simple, fabrication-friendly three-parameter lattice microstructure to realize the strongly graded and anisotropic conductivity tensors. Their approach leverages transformation thermotics, a robust framework established in 2008 for precisely controlling heat flow. Locally, a surrogate-model-based inverse homogenization maps desired principal conductivities to bar widths and covers most of the G-closure of two-phase composites. Globally, the method solves for scalar fields whose gradients align with the spatially varying principal directions, enabling an implicit wave-function plus Boolean construction of three mutually orthogonal lattice families that are smooth and naturally connected. Spherical harmonics provide analytic surface representations for complex geometries (e.g., human faces), and a near-transverse-isotropy observation enables robust regularization of ill-behaved eigenvector fields. The authors validate performance through high-resolution finite-element simulations with a relative temperature difference (RTD) metric and through experiments under multiple loading directions. The cloaks maintain straight, equidistant background isotherms and suppress core gradients for a wide range of shapes and material contrasts, outperforming many recent 2D studies while achieving substantially higher geometric complexity. Overall, the manuscript presents a comprehensive methodology with robust, well-validated results, and makes a significant contribution to advancing three-dimensional thermal metamaterials. Before I can recommend acceptance, however, a few issues should be

addressed.

1. The analysis is presented entirely for the steady-state thermal response. Could the authors provide information on the transient behavior of the system? Specifically, what is the characteristic time required for the cloak to reach thermal equilibrium after the boundary conditions are applied? A discussion on how this time scales with the cloak's size and the thermal diffusivity of the constituent materials would be insightful.

2. Following the previous point, real-world thermal environments are often not perfectly static. How robust is the cloak's performance against dynamic perturbations? For instance, after reaching a steady state, if the external heat source or sink temperature fluctuates within a small range (e.g., sinusoidal or step-wise changes), does the cloaking effect degrade? Please provide a transient simulation that tracks the Relative Temperature Difference (RTD) under such a perturbation would be a powerful demonstration of the design's practical stability and applicability.

3. The current design is optimized for a uniform background temperature gradient. How would the cloak perform if the external thermal environment was fundamentally non-uniform, such as the field generated by a point heat source placed near the cloak? Since the prescribed conductivity tensor is derived based on a uniform field assumption, some performance degradation is expected. A simulation or at least a qualitative discussion on this scenario would help define the operational limits of the proposed design.

4. The authors are commended for advancing free-form cloaking, which moves the field closer to real-world implementation. In practical scenarios, material properties can deviate from their designed values due to manufacturing inconsistencies, operational wear, or material aging. Could the authors perform a sensitivity analysis to quantify the impact of such perturbations on the cloak's performance? For example, how does the RTD change if the thermal conductivities of the AlSi10Mg and PDMS constituents vary randomly by ±5% or ±10% from their nominal values?

5. The analysis assumes perfect thermal contact at the interface between the AlSi10Mg lattice and the PDMS matrix. In a real composite, a non-zero interfacial thermal resistance will exist. Could the authors provide an estimation of the potential impact of this resistance on the cloak's performance? A brief parametric study showing the change in RTD as a function of a plausible range of interfacial resistance values would significantly strengthen the experimental claims.

6. To better situate this contribution within the developing thermal metamaterials, I suggest that the authors add a statement to a discussion section. Specifically, they should clarify how their work exemplifies and advances the "free-form" design paradigm, which was recently conceptualized in works such as Xu et al., Nature Computational Science, 4(7):532-541, 2024. The authors are to be commended for the complexity and novelty of the shapes demonstrated. While much of the prior research in transformation thermotics and metamaterials has focused on cloaking geometrically regular objects (e.g., circles, polygons), the pear and human-face shapes presented in this work are an excellent realization of a truly free-form design. This represents a significant step forward, moving the field of thermal cloaking from idealized geometries toward practical applications where objects have arbitrary and complex contours.

7. The current study masterfully addresses the thermal performance of the cloak, assuming stable material properties. However, for potential applications in high-temperature environments (e.g., aerospace, waste heat management), the thermo-mechanical integrity of the structure becomes a critical consideration. The mechanical properties of both the AlSi10Mg lattice and the PDMS matrix are known to be temperature-dependent. Could the authors please discuss the anticipated operational temperature limits of their proposed design?

8. It is anticipated that additional relevant references, including review articles and monographs, will be incorporated into the reference list to benefit readers. Additionally, a minor formatting issue has been identified in the manuscript. Specifically, units should be presented in their standard form, and a space must always be inserted between a numerical value and its corresponding unit.

Version 1:

Reviewer comments:

Reviewer #1

(Remarks to the Author)
Although several questions have been clarified, many points still remain unclear, and it is necessary to provide responses to the comments below.

Comment 1
In the reply to Comment 4 of Reviewer #1, the authors provide a table in the response letter to compare their study with previous studies. This table should be included in the manuscript to highlight the novelty of the presented study.

Comment 2
In the above table in the response letter, the authors claim that the presented method provides a "global optimum (within the achievable range)." How did the authors verify that the obtained structures correspond to a "global optimum"? The authors need to explain the method used to demonstrate the global optimality of the presented optimized structures?

Comment 3
Doesn’t the computational cost of mapping between physical property data and microstructure data largely depend on how detailed the acquisition of the physical property data and the microstructure data is?While these mapping data may be reusable, this computational cost cannot be ignored.

Comment 4
Related to the above comment, it is necessary to investigate how the resolution of the data mapping affects the optimization results. Wouldn’t these factors strongly influence the reproducibility of the results?

Reviewer #2

(Remarks to the Author)
I am fine with the implementations. It can be published.

Reviewer #3

(Remarks to the Author)
Three-dimensional thermal cloaks of arbitrary shapes hold immense application value in the infrared thermal protection of underground bunkers. This manuscript presents a comprehensive methodology accompanied by robust and well-validated results, making a significant contribution to the advancement of three-dimensional thermal cloaks, which are a representative example of metamaterials. The author has satisfactorily addressed all my queries, and I am more than willing to recommend this paper for publication in Nature Communications.

Version 2:

Reviewer comments:

Reviewer #1

(Remarks to the Author)
Since sufficient revisions and additions have been made in response to the comments, we will proceed with publication.

Response to the Editor and Reviewers

The authors are most grateful for the Editor's and Reviewers' careful reading and insightful comments and suggestions. Before the detailed response to each of the reviewer's comments, we thought it could be helpful to include a **Statement of Novelty** below to clarify the advance and the novelty of the work, as well as clearly identify the advance over our previous work.

Statement of novelty: Transformation thermotics predict the existence of 3D thermal metamaterials for omnidirectional heat manipulation. However, their realization in complex 3D space, especially, omnidirectional ones, has not been achieved thus far due to the lack of 3D design and fabrication methodologies that 1) efficiently form concise microstructures accurately delivering the wide-ranging anisotropic and spatially graded local 3D conductivity; 2) generate naturally well-connected and practically fabricable global 3D structures; and 3) are adaptable to any general and complex 3D domains.

As also confirmed by Reviewer 3's comments, our study effectively and thoroughly resolves this long-standing challenge through the following discoveries and innovations:

1) A first-time physical and experimental realization of 3D omnidirectional thermal cloaking in free-form 3D space
2) Simple 3D microstructure with large property space relative to theoretical bounds
3) Discovery of spectral properties of the 3D anisotropic conductivity space that facilitates a new strategy and high efficiency in design
4) A new 3D de-homogenization approach featuring proposed multi-step Boolean operations tailored to the graded 3D microstructure
5) The integration with spherical harmonics enabling previously unseen geometric complexity with a proposed transverse isotropy regulation

The developed method is highly general and readily extensible to other 3D thermal metamaterials predicted by transformation thermotics, such as rotators and concentrators. Hence, the developed theory and strategy fundamentally and effectively advance the field.

Advancements over previous work:

We would also like to provide additional analysis on the advancement over our previous work on 2D thermal metamaterials. The current study is a fundamental departure from the earlier 2D study for the following reasons.

1) The physical realization (fabrication & experimental reproduction) of complex-shape 3D omnidirectional cloaking is a first, to the best of our knowledge, marking a pioneering advancement in the field. Moreover, such advancement is practically unlikely to be achieved with other existing strategies due to their inability to scale. Our 2D study, on the other hand, is about creating a new and better (in efficiency, global connectivity, manufacturability) approach for 2D

omnidirectional field manipulation, which is also achievable by some other existing methods (albeit with much higher cost and lower performance).

2) The proposed 3D lattice is a discovery found based on rigorous scientific analysis independent of the previous 2D work, rather than an extension of it. The 3D lattice is created and used because of its large effective 3D anisotropic conductivity space relative to the theoretical bounds and because of its fabricability. It is fundamentally different from the 3D extension of our previous 2D laminate, which would be the 3D rank-3 laminate. In fact, we have argued and shown that such a 3D extension of the 2D laminate would not work due to its highly limited property space and inability to be 3D-printed. Hence, the proposed 3D lattice is an independent invention created with logics and analysis different from our previous 2D study.
3) This study also makes a contribution to the transformation theory, which was absent in the previous 2D study. We discovered several theoretical properties about the transformed 3D anisotropic conductivity, which were unknown previously. They include the ordering of and gaps between the three principal values, their rule of variation in space, and critical features of their principal directions. These discoveries not only mark a contribution to theoretical thermotics but also facilitate the dimension reduction in subsequent engineering design, which greatly reduces the design cost. These properties and techniques critical to the 3D cloak are absent and not needed in the 2D cloak (previous work).
4) The 3D de-homogenization tailored to the 3D lattice is fundamentally new because of the proposed multi-step Boolean operation, and it is not a 3D extension of the previous or existing 2D approach. Existing de-homogenization techniques can mostly represent plate-like 3D structures or laminate-like 2D structures (previous study), which lack the multi-step Boolean operation required to form the 3D bar-like lattice with the three independently varying cross-sectional areas.
5) The novel integration of transformation thermotics with spherical harmonics and a proposed transversely isotropic regularization enables the design of thermal metamaterials with geometric complexity far exceeding that of our previous 2D studies and indeed any existing studies on 2D metamaterials. It also marks a new record in geometric versality of fabricable 3D omnidirectional thermal metamaterial.

Response to the reviewers

The authors are most grateful for the Reviewers' careful reading and insightful comments and suggestions. We have thoroughly revised the main manuscript and Supplementary Information according to all the comments. The point-to-point response is highlighted in **blue**, and the corresponding changes in the revised manuscript and Supplementary Information are highlighted in **red**. Below we address each comment in detail.

Reviewer #1 (Remarks to the Author):

This paper employs transformation theory and de-homogenization to investigate the design and practical application of a three-dimensional thermal cloaking system composed of three-dimensional lattice microstructures. Based on collected data on homogenized thermal conductivity, the authors optimize the size of the microstructures to achieve the desired anisotropic thermal conductivity and position them accordingly to design the overall structure. Because the entire structure is designed theoretically, full-scale simulations are not required, and the computational cost may appear low. However, in practice, the size of each microstructure is optimized for every spatial location, and when data collection for homogenized thermal conductivity is included, the computational cost increases accordingly. The obtained numerical results are impressive, and the resulting structure is intriguing. Nevertheless, given the claimed methodological advances and their apparent effectiveness, it remains unclear whether this paper meets the publication standards of Nature Communications (though this reviewer's overall impression is not negative). This reviewer will consider the authors' revisions and responses to the comments below before deciding whether to recommend publication.

We sincerely thank the reviewer for the comments. We have addressed them point-by-point, and the corresponding manuscript revisions are included in this file in red.

Regarding the reviewer's concern about the computational cost, we would like to provide a summarized explanation/clarification here that the reported time is indeed the total time needed to create any new 3D metamaterial with our approach. The *parameter identification* of the 3D microstructures in space does not involve numerical homogenization because it is performed based on a precomputed and prestored database, and hence it is carried out very efficiently. The database is metamaterial-independent, and it is constructed only once and stored for the design of any new 3D metamaterial. The detailed analysis and evidence are provided in our later response to the reviewer's comment on computational cost. To avoid the potential confusion/conception that numerical homogenization is required for the microstructure design, we have changed "inverse homogenization" and "inverse design" to "parameter identification".

1. Is the main significance of this paper that it extends the authors' previous theory from their Nature Communications paper [10] to a three-dimensional system? Theoretical constructs such as de-homogenization, transformation thermotics, and the wave function expression are again employed in the present study, suggesting that theoretical progress may be limited.

We thank the reviewer for the important question. Regarding the novelty of this paper, we would like to provide the following clarification and also refer to the statements by Reviewer 3 on page 19 and the summarized "Advancements over previous work" in pages 1-2.

We wish to clarify and demonstrate that the advancement to 3D cloaks is neither marginal nor straightforward. It is only made possible by several new findings in theory and methodology. First, the rank-N laminate that performs very well in 2D does not work in 3D due to its very limited property range and difficulty in fabrication caused by its closed spaces, as revealed in the SI 4.2. We discovered that the parameterized 3D lattice structure covers the physically admissible anisotropic conductivities needed by transformation thermotics, which is an important observation unrevealed previously. This is also the main rationale for adopting this 3D microstructure. Second, we discovered/proved several important spectral properties of the 3D conductivity tensor (SI 3) that are absent in 2D and also previously unknown. These properties enable and inspire a dimension-reduction strategy for designing 3D thermal metamaterials defined by the surface of revolution, which significantly reduces computational cost down to a 2D problem, and avoids the expensive brute-force solution. Such a theory-enabled 3D design process was previously unknown. Third, we fundamentally modified the global wave-function in the de-homogenization with newly developed and non-intuitive multi-step Boolean operations that enable an accurate global representation of the spatially graded 3D lattice. 3D de-homogenization with this capacity and compatible with the proposed 3D lattice has been absent to the best of our knowledge, and the innovations therein significantly depart from the 2D de-homogenization. Fourth, we proposed the integration between transformation thermotics and spherical harmonics, which allows for the record-breaking geometric complexity of the 3D human-face cloaks unseen in thermal metamaterials. Fifth, we proposed a transverse isotropy regularization approach that enables desired modification of non-smooth eigenvector fields without significant performance deterioration, improving fabricability while achieving the complex human-face cloaking. These theoretical advancements are fundamentally new from the 2D setup and indeed unseen in the field, and they are highly general/transformative in that they readily apply to other 3D conductive metamaterials.

Additionally, it is the above theoretical advancement that enables the practical fabrication of free-form 3D thermal metamaterial and experimental reproduction of omnidirectional 3D cloaking in a highly complex 3D space. To the best of our knowledge, this current manuscript is a first (the 3D cloaking in *Nature Computational Science, 4(7):532-541, 2024* is non-omnidirectional), which is scientifically significant to the field of thermal metamaterials.

To better convey our theoretical/methodological innovations in the main text, we have revised the manuscript as follows.

In the third paragraph of the introduction:

"… This is achieved by leveraging special spectral properties of the transformed 3D conductivity and integrating a new 3D de-homogenization method [46-50] with a functionally robust yet geometrically simple, 3D lattice microstructure…."

"…With a proposed integration of 3D de-homogenization with spherical harmonics -- the Fourier transform on a sphere -- and a transverse isotropy regularization technique, we achieve 3D thermal cloaks with unprecedented geometric complexity, such as the shape of a human face, while still exhibiting excellent thermal cloaking. The findings resolve the fundamental challenge of realizing 3D transformation thermotics, creating a practical route for engineering wide-ranging advanced 3D thermal meta-devices as well as other 3D conductive systems, such as electrical conduction and pressure flow.”

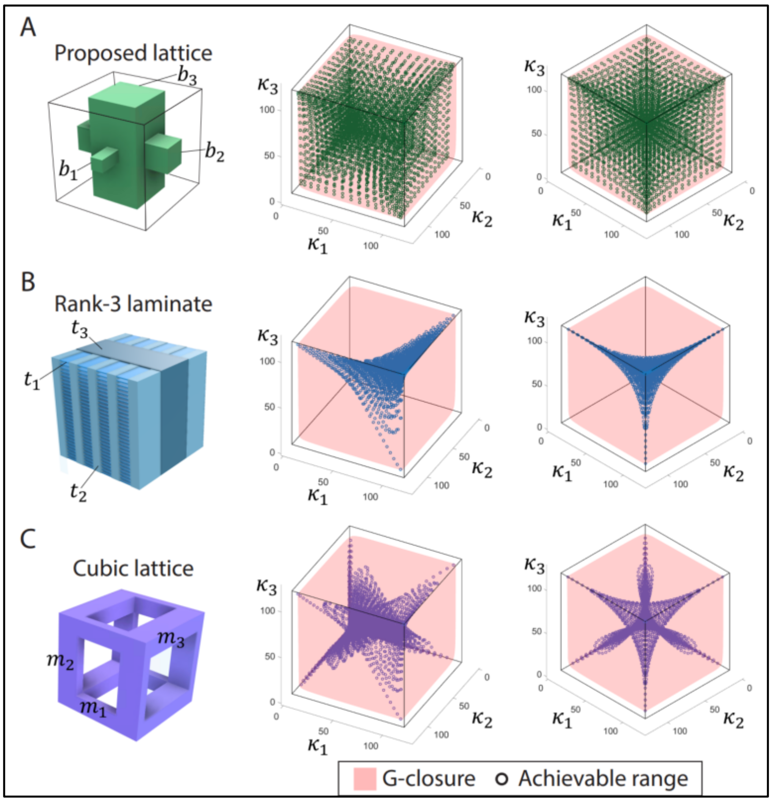
We also added a discussion section at the end of the main text, summarizing our key contributions:

“This study demonstrates a precise, efficient, and practical design-fabrication strategy for realizing omnidirectional, arbitrary-shaped 3D thermal meta-devices predicted by transformation theory. This is made possible by 1) the discovery of special spectral properties of the transformed 3D conductivity that significantly accelerates the subsequent design process; 2) the proposed geometrically simple 3D lattice microstructure with the required large effective property space; 3) a new 3D de-homogenization technique featuring multi-step Boolean operations tailored to the 3D lattice; and 4) the integration of transformation thermotics with spherical harmonics aided by a proposed transverse isotropy regularization.

The combined method enables the creation of 3D thermal meta-device structures that are locally concise, naturally well-connected, capable of adapting to highly complex domains, and practically fabricable. Regardless of the geometry, the 3D thermal cloaks demonstrate great performance in concealing objects under multi-directional thermal detection, as evidenced by their small RTD indexes. With metal 3D printing, we accurately fabricate the 3D thermal cloak and successfully reproduce the omnidirectional cloaking effect in experiments.

The findings provide a competitive and general solution to the long-standing challenge of accurately realizing 3D graded and anisotropic material properties. They also advance the field of thermal metamaterial from idealized 2D geometries toward practical applications, where objects have arbitrary and complex 3D geometries. The developed methodology is general and transformable, readily extensible to other 3D thermal and conduction-dominated meta-devices across various disciplines.”

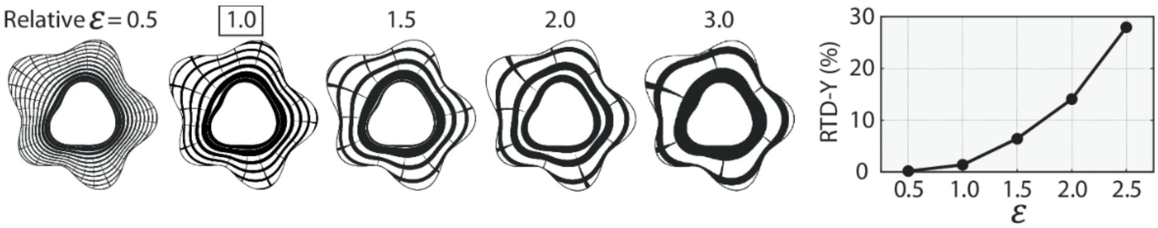
2. It is unclear what the widths b_1, b_2, and b_3 refer to. Please indicate these clearly in the figure showing the microstructure in the supplementary material.
   We thank the reviewer for pointing this out. They are added to SI Figure 1 as shown below. The parameters of the other two microstructures are also added. We also changed the illustration of the rank-3 laminates to a more accurate representation comprised of lamination in three different scales.



3. The characteristic size of the microstructure appears comparable to the macroscopic dimensions, which raises concerns about the validity of the scale separation assumption in the de-homogenization procedure. I recommend providing quantitative evidence or discussion to confirm that scale separation is satisfied. In addition, please identify and illustrate the Representative Volume Element (RVE) used in your analysis and clarify how it represents the overall microstructural behavior.

We thank the reviewer for raising this point. We have performed an investigation on the convergence of feature size in our earlier study on 2D thermal cloaks *W. Li et al. Nat. Commun. 15 (1), 5527* as shown in the attached plot below. While smaller feature size generally produces better performance, the selected fabrication-friendly feature size (the second from the left in the figure below) can already accurately achieve the omnidirectional cloaking, with RTD values lower than 1.4%. The current study on 3D thermal cloak adopts a similar microstructural feature size relative to the overall scale of the metamaterial, and the demonstrated small RTD values in three different directions suggest that the current feature size is indeed valid.

We also remark that separation of scales is less of an issue for de-homogenization as observed in several works. The microstructures are by construction optimally aligned with principal stresses (elasticity) or thermal gradients (thermal cloaks) and thus computed homogenized properties are highly accurate, even for coarse scale realizations.



We have added a comment on the feature size before Section 2 in the revised main text as attached below.

"Also, the current microstructure feature size is a balance between separation of scale and fabricability but achieves great cloaking performance while remaining practically fabricable, as demonstrated next."

Regarding the comment on RVE, we would like to clarify that this study did not adopt the standard RVE method where the domain is partitioned into periodic unit cells in which the microstructure is designed and then assembled back into the global structure. Rather, the global structure is directly mapped through a pseudo-conformal mapping with guaranteed smooth connectivity, which is why the global structure is free of the cellular voxel texture in structures produced by RVE methods. The study adopts numerical homogenization in the construction of the microstructure's surrogate model of the homogenized properties (we noted that once the surrogate model database is created, the creation of any new 3D metamaterial and the parameter identification of the 3D microstructures in space does not involve numerical homogenization because it is performed based on a precomputed and prestored database, please see response above in Page 3). We have added the details on the numerical homogenization in the revised SI 4.1, as attached below.

"The 3D lattice does not have a closed-form formula for its homogenized conductivity, and we adopt a surrogate model constructed based on off-line numerical homogenization. Here, we provide the relevant details. For the off-line numerical homogenization, we focus on one unit cell with parameters b_i and follow the standard procedure as described below. For a unit cell with local coordinate denoted as $\boldsymbol{y}$, the effective/homogenized conductivity $\boldsymbol{\kappa}$ is evaluated through

$$\boldsymbol{\kappa} = \int_{\mathrm{Y}} \hat{\boldsymbol{\kappa}}(\boldsymbol{\delta} - \nabla\boldsymbol{\xi})\mathrm{d}V$$

where $\hat{\boldsymbol{\kappa}}$ is the local constituent's conductivity tensor, $\boldsymbol{\delta}$ is Kronecker's delta (identity matrix), Y denotes the unit cell domain, ∇ denotes the gradient, and vector $\boldsymbol{\xi}$ is obtained as follows. Let scalar field $\gamma = \boldsymbol{E}\cdot(\boldsymbol{y}-\boldsymbol{\xi})$ where $\boldsymbol{E} = [1,0,0]$ or $[0,1,0]$ or $[0,0,1]$ is the probing vector in the principal frame. The γ is obtained by solving the following PDE (source-free heat equation)

$$\nabla\cdot(\hat{\boldsymbol{\kappa}}\nabla\gamma) = 0$$

subjected to periodic boundary conditions $\gamma^{(q)} - \gamma^{(p)} = \boldsymbol{E}\cdot\left(\boldsymbol{y}^{(q)} - \boldsymbol{y}^{(p)}\right)$, where $\nabla\cdot$ denotes the divergence, and p and q denote periodic pairs of the unit cell's boundary.

Equation (26) is solved using FEM with a $64 \times 64 \times 64$ structured mesh. The problem is solved for the three probing vectors, resulting in the corresponding three γ fields, with which we can compute $\boldsymbol{\xi}$ and then evaluate the homogenized $\boldsymbol{\kappa}$ using equation (25). As the FE coordinate frame aligns with the microstructure's principal frame, the obtained $\boldsymbol{\kappa}$ is in diagonal form with three principal values κ_i.

Based on the above numerical homogenization, we construct the surrogate model of $\boldsymbol{b} \rightarrow \boldsymbol{\kappa}$ off-line via a parameter sweep of $b_i \in [0,1]$, which is equally discretized into 32 intervals, and the corresponding homogenized κ_i are collected. Making use of symmetry, we can reduce the number of evaluations to 1/6 of the full permutation [2]. Additionally, we also compute the gradient information of $\partial\kappa_i/\partial b_j$ using 3-point central difference based on the $\boldsymbol{b} \rightarrow \boldsymbol{\kappa}$ database and store them for the later numerical parameter identification."

4. Although the proposed method is claimed to outperform other thermal cloak design approaches, particularly topology optimization, the comparison presented in the introduction is not sufficiently comprehensive. Please include a more detailed comparison of the various methods available for designing thermal cloaks, discussing their respective advantages, limitations, and computational costs.

   We thank the reviewer for raising this point. The scope of this study is free-form 3D omnidirectional thermal metamaterials generated based on transformation thermotics. We could not find any other study with the same scope for a fair and quantitative comparison (the study *Nature Computational Science, 4(7):532-541, 2024* is non-omnidirectional). There are a few studies focusing on 2D free-form omnidirectional thermal metamaterials, which use a "divide and conquer" strategy that partitions the design domain into many unit cells. Each unit cell is filled with a free-form microstructure generated by topology optimization (*Nat. Commun., 12(1):7228, 2021*) or a trained neural network (*Advanced Materials, 35(33):2302387, 2023*). In the following, we present a discussion and qualitative evaluation of these strategies relative to our method. The comparison is summarized in the table below.

	Divide & Conquer + TO microstructure (e.g., *Nat. Commun., 12(1):7228, 2021*)	**Divide & Conquer + AI microstructure** (*Advanced Materials, 35(33):2302387, 2023*)	**This study**
Dimension	2D	2D	**3D**
Direction dependence	Omnidirectional	Omnidirectional	Omnidirectional
Microstructure global optimal	Local due to non-convexity	Local due to non-convexity	Global optimum (within achievable range)
Microstructure inverse design cost	Very high cost, each unit cell needs a 3D TO process with numerical homogenization (quantitative computational cost not disclosed)	Not demonstrated in 3D, but presumably low-cost after potentially expensive training (quantitative computational cost not disclosed)	Low cost (~22 mins) thanks to geometric simplicity & surrogate model (~0.8 s each per computation core)
Global structure generation	Unit cell assembly	Unit cell assembly	3D de-homogenization with multi-step Boolean operations
Global 3D connectivity	Not demonstrated in 3D, but based on the 2D version, heavy post-processing should be required	Not demonstrated in 3D	Naturally guaranteed without post-processing
Global structure fabricability	Not demonstrated in 3D, but the high complexity in 3D microstructure would be very challenging to fabricate	Not demonstrated in 3D, but the high complexity in 3D microstructure would be very challenging to fabricate	Practically fabricable as demonstrated
Cloaking performance in RTD	Not demonstrated in 3D nor reported in 2D	Not demonstrated in 3D, the 2D reported values of free-form geometry are 0.13 - 0.39	RTD in 3D with similar geometric complexity is 0.03 - 0.15

We have added a subsection in SI 8 to discuss the above analysis, as shown in the following.

“We provide a qualitative comparison and assessment of some of the latest methods for designing free-form omnidirectional thermal meta-devices with transformation thermotics. Methods for non-omnidirectional performance or non-free-form geometries are beyond the scope of our discussion. The main strategies other than the current method for designing 2D free-form thermal meta-device adopt a ``divide-and-conquer'' strategy, where the domain is partitioned into many square-shaped unit cells, and their microstructures are designed with topology optimization (TO) [16, 17, 18] or artificial intelligence (AI) [19], and the microstructures are later assembled back to the meta-device. These methods have produced fabricable thermal meta-devices in the 2D setup, but have not been used in the design of free-form 3D meta-devices. Here, we provide a speculative analysis of these methods in the 3D design setup and compare them to this study's method.

For the design of 3D (and 2D) microstructures, free-form microstructures designed by TO or AI generally have no guarantee to attain the global optimum due to non-convexity of the design problem. By contrast, the proposed 3D lattice has only three design variables, and the parameter-property mapping is one-to-one as demonstrated by the property space plot in Figure 1 A, except for the extreme isotropic point of κ_A. The global optimum is therefore reachable for the proposed method.

In terms of computational cost, the TO-based method is very expensive as each 3D unit cell needs a 3D topology optimization consisting of at least hundreds of thousands of design variables and typically hundreds of optimization steps, each of which require solving three FEA in the numerical homogenization process. The AI-based method should significantly accelerate the microstructural design process after the neural network is trained albeit through a potentially expensive process. The method proposed here is highly efficient thanks to the three-parameter microstructure and surrogate model. As shown in the previous section, the design cost for one unit cell is about 0.05 seconds via 16-core parallel computation (or 0.8 s per computer core).

Regarding 3D global connectivity, the TO-based method would require heavy post-processing as evidenced in its 2D application [16. 17, 18]. The challenges of post-processing 3D connectivity would be significantly greater than 2D and degrade the performance. The AI-based method trained with selected TO-generated microstructures should exhibit improved connectivity, although whether such an advantage can be generalized to 3D microstructures remains unclear. Our proposed method naturally guarantees global connectivity thanks to the continuous and smooth pseudo-conformal mapping and 3D de-homogenization.

For fabricability, both the TO- and AI-based methods tend to generate highly complex microstructures that can be challenging to fabricate in a general 3D setup. In particular, the microstructures need to be free of closed spaces for powder-bed metal 3D printing, and the overall structure needs to be simple enough for workability, such as support removal. It is unknown how these requirements can be efficiently and systematically met by the TO- and AI-based methods. The proposed 3D lattice is simple in geometry and free of closed spaces, and the global structure is practically fabricable as demonstrated."

5. Related to the above point, potential reviewers may wish to see how the computational cost of this approach compares with other methods (e.g., topology optimization). A fair comparison should include all relevant computational efforts, including preparatory steps such as the collection of homogenized thermal conductivity data.

We thank the reviewer's suggestion. We wish to clarify that there seems to be no design methods in the literature that tackle free-form 3D omnidirectional thermal metamaterials based on transformation thermotics. We therefore could not compare in a fair way. For the cited studies with free-from 2D thermal metamaterials (topology optimization or AI), their computational costs are not disclosed. We would therefore present the computational cost of our approach using a representative Dsg. 4 of the main text Figure 3, which is a general 3D shape. The computational cost mainly consists of three parts: 1) nonlinear finite-element solution for the pseudo-conformal mapping; 2) microstructure parameter identification based on the surrogate model; 3) design generation. We wish to clarify that the collection of homogenized thermal conductivity should not be counted as design cost because it is performed once and stored for future design of any new 3D thermal metamaterials.

Based on the above setup, using a workstation with AMD EPYC 7K62 96-Core Processor 2.60 GHz (actual use of 16 cores) and 256 GB RAM and Matlab 2025b, the cost profile of the Dsg.4 thermal cloak is as follows.

1) Solution for pseudo-conformal mapping (including FE meshing and nonlinear solution): 235.1 s
2) Microstructure parameter identification (27864 microstructures): 1333.8 s (~22 mins)
3) Design generation (resolution 576 x 576 x 576): 51.8 s

Hence, the total computational cost of generating a free-form 3D thermal cloak is 27 mins. The 1333.8 s of parameter identification suggests that each microstructure takes 0.05 s (or 0.8 s per core) on average. This would significantly outperform a topology optimization approach, which performs a 3D topology optimization consisting of at least hundreds of thousands of design variables with typically hundreds of iterations, each of which requires solving three large linear systems in the numerical homogenization.

We have added the above information in the SI 7 of the revised manuscript as attached below.

"The computational cost for generating a global cloaking structure consists of three parts: 1) the nonlinear FE solution of the pseudo-conformal mapping, 2) the parameter identification based on the surrogate model, and 3) global structure generation. The cost of building the 3D lattice's surrogate model is not included in the design cost because it is design-independent and needs to be computed only once and then stored for the design of any other thermal meta-devices.

Here, we report the computational cost of a representative Dsg.4 in the main text Figure 3, which has a general 3D shape. We use a 64 x 64 x 64 base structured mesh with those in the background and core regions removed. Using a workstation with AMD EPYC 7K62 96-Core Processor 2.60 GHz (actual use of 16 cores) and 256 GB RAM, the computational costs are: 1) 235.1 s for nonlinear FE solution of pseudo-conformal mapping, 2) 1333.8 s for the parameter identification of 27864 microstructures (0.05 s for each microstructure), and 3) 51.8 s for structure generation with 576 x 576 x 576 pixels. We note that for 3D domains defined by surfaces of revolution, the computational cost can be significantly reduced for the pseudo-conformal mapping solution and parameter identification. Also, further cost reduction can be achieved by special programming techniques such as mixed programming with the C language."

6. Thermal conductivity should be expressed in units of W/(m·K) rather than W/mK to make it clear that the kelvin unit is in the denominator.

   We thank the reviewer's suggestion. All units are corrected.

7. The paper's tone is sometimes overly laudatory, with phrases such as ``elegant and general transformation theory'' that obscure the main message. Unless these are technical terms, please revise such expressions throughout the manuscript to maintain a more neutral and objective tone.

   We thank the reviewer's suggestion. A neutral and objective tone is now used in the revised manuscript.

Reviewer #2 (Remarks to the Author):

This manuscript realizes three-dimensional thermal cloaking with arbitrarily complex shapes via a 3D lattice composite. Numerical and experimental results both verify good thermal manipulation performances. Unfortunately, I do not recommend it for publication due to lacking novelty. The progress on realizing a 3D cloak with arbitrary 3D space is not interesting enough to publish in a journal like Nature Communications. Some specific concerns are listed below.

We thank the reviewer's comments, and have addressed them point-by-point. The corresponding manuscript revisions are attached in this file in red.

1. Page 1. I do not agree with the claim "Real-world applications are three-dimensional, and how to realize the elegant transformation theory in a general 3D domain and engineer free-form 3D omnidirectional thermal meta-devices remains far from being understood." Is transformation thermodynamics not understood in general 3D domain? There are a lot of works on that. Cloaks with complicated shapes were extensively studied in the field of electromagnetism and acoustics (1-7). They were later transferred to heat diffusion fields (8-10). Han et.al. and Liu et.al. designed arbitrarily polygonal cloaks with homogeneous and non-singular parameters (11-12). Xu et. al. designed arbitrary polygonal thermal schemes using the linear mapping functon(13-16).

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3) W. X. Jiang, J. Y. Chin, Z. Li, Q. Cheng, R. Liu, and T. J. Cui, Phys. Rev. E, 2008, 77, 066607.
4) H. Ma, S. Qu, Z. Xu, and J. Wang, Opt. Express, 2008, 16, 15449-154454.
5) M. Rahm, D. Roberts, J. Pendry, and D. Smith, Opt. Express, 2008, 16, 11555-11567.
6) G. Zhu, J. Appl. Phys., 2013, 113, 163103.
7) Q. Li and J. S. Vipperman,Appl. Phys. Lett., 2014, 105, 101906.
8) T. H. Li, D. L. Zhu, F. C. Mao, M. Huang, J. J. Yang, and S. B. Li, Front. Phys., 2016, 11, 110503.
9) Peralta and V. D. Fachinotti, Sci. Rep., 2017, 7, 1-8.
10) X. Wang, S. Qu, X. Wu, J. Wang, Z. Xu, and H. Ma, J. Phys. D: Appl. Phys., 2010, 43, 305501.
11) T.Han, C. Qiu, and X. Tang, J. Optics, 2010, 12, 095103.
12) Y.Liu, W. Guo, and T. Han, Int. J. Heat Mass Transfer, 2017, 115, 1-5
13) G. Xu, H. Zhang, and Y. Jin, Energ. Convers. Manage., 2018, 165, 253-262.
14) G. Xu, X. Zhou, and Z. Liu, Int. Commun. Heat Mass, 2019, 108, 104337.
15) Q. Li and J. S. Vipperman, J. Appl. Phys., 2018, 124, 035103.
16) Q. Ji, et al. ES Energy Environ., 2020, 7, 29-39

Regarding novelty of this paper, we would like to provide the following remarks and also refer the

Reviewer 2 to the statements by Reviewer 3 in page 19. We furthermore read each of the 16 papers that Reviewer 2 mentioned and have carefully marked the differences and confirmed that none of the work has a physical/experimental realization of a cloak and they are theoretical and numerical, most of which assume continuous and unrealized materials (please see the table of summary of key comparison below).

We wish to clarify that the novelty of this work lies in the engineering dimension, including structural design theory and strategy, fabrication, and experimental validation, and not in the theoretical transformation physics suggested in the comment. This scope has been consistently presented throughout the manuscript. The reviewer's question "Is transformation thermodynamics not understood in general 3D domain?" is therefore not related to this manuscript's scope, and we did not claim or suggest that transformation thermodynamics is not understood.

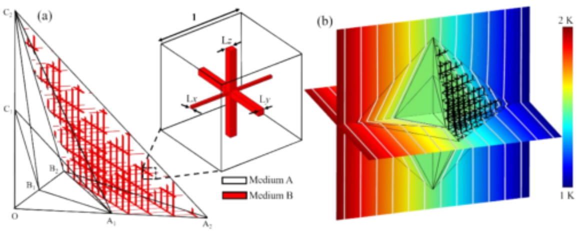
Our claim of "how to realize free-form 3D cloaks in 3D space remains unclear" refers to the efficient generation of fabricable and globally well-connected 3D structures for the accurate attainment of complex 3D anisotropic conductivity distribution and the physical realization (fabrication + experiment) of the omnidirectional 3D cloaking in highly complex 3D space. To the best of our knowledge (including the reviewer's cited works), this is not well understood and has not been achieved thus far (based on general transformation theory), and it is effectively resolved in our work.

We do not find that the papers cited by the reviewer suggest that our innovation is marginal or already achieved. Instead, they effectively show that our innovation is novel and significant for the following reasons.

1) All the cited studies are numerical or theoretical, and none involve fabrication or experimental realization. The departure from purely theoretical/numerical designs to physical 3D structures that are theoretically accurate, efficient to generate, globally well-connected, adaptable to any complex shapes, and practically fabricable is not marginal. It is facilitated by a number of theoretical and methodological innovations achieved in our study. Additionally, the successful physical reproduction of the free-form 3D omnidirectional cloaking designed based on transformation theory is, to the best of our knowledge, a first, which is a significant advancement in the field of thermal metamaterials.
2) Most of the cited papers that includes numerical/theoretical microstructures adopt the layered structures (2D and 3D rank-1 laminate Ref. [6-9, 12-14]), but they are neither theoretically accurate (rank-1 laminates produce a de-generated and highly limited property space) in producing the wide-ranging anisotropic conductivity, nor are they straightforwardly fabricable in the free-form 3D setup as they form closed chambers that are hard to 3D-print with metal. Some numerical studies use rank-1 laminates with 3-4 different base material layers, which makes it even more difficult to fabricate in the 3D setup. The paper Ref. [16] uses the same

form of 3D microstructure as ours, but limited to polyhedral shapes far simpler than required for the human-face geometry achieved in our study, and no actual fabrication is carried out. Also, the important information of the microstructure's property space (achievable range of anisotropic conductivities) relative to the theoretical bound is not revealed or discussed. Moreover, Ref. [16] did not answer or address how to adapt the microstructure to general 3D shapes beyond polyhedra, which requires spatial alignment with complex principal directions while ensuring connectivity. This is not a straightforward process achievable via existing approaches. These fundamental design challenges are resolved in our study through the discoveries in the spectral properties of conductivity and the new 3D de-homogenization technique. The above observations suggest that there is a lack of knowledge in this field on what type of microstructure works well theoretically and practically for the challenging free-form 3D thermal metamaterial, and how to effectively assemble the microstructures into a well-connected and fabricable global design. These fundamental scientific challenges involving composite theory, design, and fabricability are effectively addressed by our study.

3) The level of 3D geometric complexity achieved in the cited papers does not match that of our cloak. The most complicated 3D shapes among the cited papers are composed of polyhedra, far less complicated compared to our multi-human-face cloak. Moreover, the polyhedral shape is a requirement by the applied linear mapping method rather than a choice, implying a restriction on the form of 3D shapes. By contrast, our study imposes no limitations on the shape of the thermal metamaterial as demonstrated by the 3D human-face cloak.
4) The cited papers involving microstructures did not answer the important question of how to ensure fabricability in the free-form 3D setup. For example, although Ref. [16] proposes the local form of the lattice microstructure, it did not answer how to lay out or assemble the lattices globally in a fabricable way to form 3D cloaks with complex shapes.
5) It is unclear whether the linear mapping and polyhedral setup in Ref. [16] and others can be used for other thermal metamaterials (such as rotators) with different transformation rules. Whether the property of locally homogeneous blocks required for the regular layout of the 3D lattice in [16] would remain valid for other metamaterials is unknown. By contrast, the pseudo-conformal mapping and 3D de-homogenization developed in our study is highly general and can readily be applied to any transformation-based thermal metamaterials, such as rotators, concentrators, camouflages, etc.



The above observations and analysis demonstrate that our innovations in design theory/methodology as well as a first physical reproduction of free-form omnidirectional 3D cloaking mark a significant advancement in the field of thermal metamaterials.

A summary of key information in the papers cited in the comment is attached below as supporting information.

Paper no.	Dimension & geometry	With microstructures?	Form of microstructure	Fabrication & experiment?
1	2D - free form	No		No
2	2D/extruded - free form	No		No
3	2D - free form	No		No
4	2D - free form	No		No
5	2D - free form	No		No
6	2D - free form	**Yes**	Rank-1 laminate	No
7	2D - free form	**Yes**	Rank-1 laminate	No
8	**2D & 3D-polygonal/polyhedral**	**Yes**	Rank-1 laminate (layered with 4 base materials)	No
9	2D - free form	**Yes**	Rank-1 laminate	No
10	2D-polygonal	No		No
11	2D-polygonal	No		No
12	2D-polygonal	**Yes**	Rank-1 laminate (layered with 4 base materials)	No
13	2D-polygonal	**Yes**	Rank-1 laminate (layered with 3-4 base materials)	No
14	2D-polygonal	**Yes**	Rank-1 laminate (layered with 3-4 base materials)	No
15	**3D-polyhedral**	No		No
16	**2D & 3D-polygonal/polyhedral**	**Yes**	Rank-1 laminate (layered with 3-4 base materials) **3D lattice**	No

We have added the citation of Ref. 8, 15, and 16 to the revised Introduction as follows.

"The majority of existing studies in 3D are theoretical and numerical [27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37], most of which assume continuous and physically un-realized materials."

2. Besides, 2D omnidirectional thermal meta-devices has been studied. They are also mentioned by the authors, such as references [9] [11] [16] [22] [24]. Why to claim “engineer free-form 3D omnidirectional thermal meta-devices remains far from being understood”? What exactly is far from being understood? Is there any different principle or any paradigm shift when extending from 2D to 3D? To me, the 3D case is simply more complex, labor-cost and time consuming, while shows no fundamental difference with 2D case in the design principle. Related with the first question, what is the main contribution of this work? Is it an incremental progress from 2D to 3D? what is the novel design principle or new avenue here? Without such highlighted novelty, the manuscript is not convincing to publish in Nature communications.

We respectfully disagree that the extension from 2D to 3D is simple or incremental, as explained in the comment. From the design and engineering perspectives, generalization to 3D is highly non-trivial and fundamentally different from 2D for the following reasons (and as shown in the table above, the physical realization of 3D freeform omnidirectional cloak is not yet achieved).

In the design dimension, direct and brute force extension of popular 2D design methods (such as topology optimization and AI-generated free-form designs in *Nat. Commun., 12(1):7228, 2021* and *Advanced Materials, 35(33):2302387, 2023*) to 3D is practically prohibitive because: a) design cost increases by several orders of magnitudes; b) connectivity of 3D microstructures made of 3D bars, shells and blocks cannot be guaranteed and would be extremely hard and expensive to post-process without significant deterioration in local effective properties; c) unlike 2D, free-form 3D microstructures generated by AI or topology optimization are hardly fabricable due to the extreme complexity and potentially closed spaces. These basic facts show that the direct/brute-force extension of popular 2D approaches to 3D, as suggested in the comment, is infeasible from the initial design stage, much less for fabrication.

Our new approach is free of the above issues precisely because of the innovation in the design theory/method, which include: a) simple microstructure with 3 local design variables and disclosure of their robustness in property space; b) theoretical discovery of the special spectral properties of transformed conductivity that allow for dimension reduction for some 3D domains; c) 3D pseudo-conformal mapping and a new 3D de-homogenization approach featuring multi-step Boolean operations that generate global structures preserving 3D asymptotic properties and naturally ensuring connectivity; and d) integration with spherical harmonics and the development of a transverse isotropy regularization enabling the structural realization of 3D metamaterials with record-breaking geometric complexity. These innovations in 3D design theory/methodology are non-trivial.

In addition to the design dimension, the fabrication and a first physical reproduction of transformation-based 3D omnidirectional cloaking in complex 3D space are also scientifically significant. They demonstrate that omnidirectional heat manipulation in 3D space can indeed be practically realized. To the best of our knowledge, this has not been achieved thus far.

To better convey the above innovations and advancements, we have revised the last paragraph of the Introduction as shown below.

"… This is achieved by leveraging special spectral properties of the transformed 3D conductivity and integrating a new 3D de-homogenization method [46-50] with a functionally robust, yet geometrically simple, 3D lattice microstructure…."

"…With a proposed integration of 3D de-homogenization with spherical harmonics -- the Fourier transform on a sphere -- and a transverse isotropy regularization technique, we achieve 3D thermal cloaks with unprecedented geometric complexity, such as the shape of a human face, while still exhibiting excellent thermal cloaking. The findings resolve the fundamental challenge of realizing 3D transformation thermotics, creating a practical route for engineering wide-ranging advanced 3D thermal meta-devices as well as other 3D conductive systems, such as electrical conduction and pressure flow."

We have also added a discussion section to the end of the revised manuscript as follows.

"This study demonstrates a precise, efficient, and practical design-fabrication strategy for realizing omnidirectional, arbitrary-shaped 3D thermal meta-devices predicted by transformation theory. This is made possible by 1) the discovery of special spectral properties of the transformed 3D conductivity that significantly accelerates the subsequent design process; 2) the proposed geometrically simple 3D lattice microstructure with the required large effective property space; 3) a new 3D de-homogenization technique featuring multi-step Boolean operations tailored to the 3D lattice; and 4) the integration of transformation thermotics with spherical harmonics aided by a proposed transverse isotropy regularization.

The combined method enables the creation of 3D thermal meta-device structures that are locally concise, naturally well-connected, capable of adapting to highly complex domains, and practically fabricable. Regardless of the geometry, the 3D thermal cloaks demonstrate great performance in concealing objects under multi-directional thermal detection, as evidenced by their small RTD indexes. With metal 3D printing, we accurately fabricate the 3D thermal cloak and successfully reproduce the omnidirectional cloaking effect in experiments.

The findings provide a competitive and general solution to the long-standing challenge of accurately realizing 3D graded and anisotropic material properties. They also advance the field of thermal metamaterial from idealized 2D geometries toward practical applications, where objects have arbitrary and complex 3D geometries. The developed methodology is general and transformable, readily extensible to other 3D thermal and conduction-dominated meta-devices across various disciplines."

3. In Fig.1, the local microstructure and its effective conductivity have been well described in

literature (Q. Ji, et al. ES Energy Environ., 2020, 7, 29-39) which is based on two-scale homogenization method. In their works the parameters of such structures were also optimized to design 3D thermal cloaks. In this manuscript the authors employ identical microstructures and similar design process, without citing this work and without showing any advantage over the published work.

We thank the reviewer for pointing out this paper. We would like to clarify that our discovery of the 3D lattice microstructure is independent of *ES Energy and Environment, 7:29–39, 2020*, and it is chosen because of its broad coverage of admissible anisotropic conductivities relative to the theoretical bounds as demonstrated by our analysis. This important theoretical insight is not studied or revealed in *ES Energy and Environment, 7:29–39, 2020*. Another reason for choosing this microstructure is that it is free of closed chambers that would be hard to fabricate by 3D printing. Such a manufacturing aspect was not revealed in *ES Energy and Environment, 7:29–39, 2020* either.

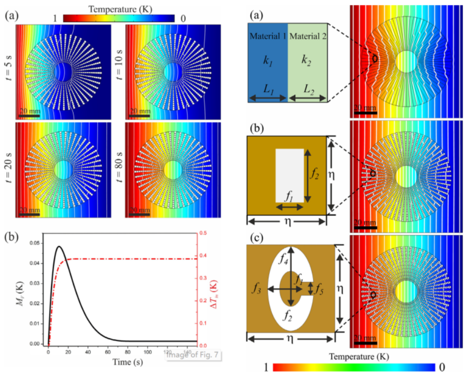
In the global dimension, we developed a new 3D de-homogenization approach tailored to the 3D lattice that enables smooth, graded, and well-connected overlay of the microstructure to arbitrarily complex domains while preserving the lattices' effective properties. Such local-to-global mapping required for adaptation to general complex domains other than polyhedra, as well as to other thermal metamaterials, is not developed in the cited paper. Finally, the cited study is purely numerical and did not fabricate or validate the thermal metamaterial.

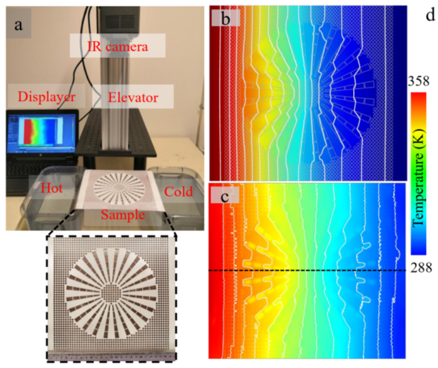
We have cited this work in the second paragraph of Sec. 1 of the revised main text as follows.

"The lattice's coverage of the conductivity parameter space is also much greater than that of some other simple microstructures such as rank-3 laminates, which achieve more extreme properties but in a smaller parameter range (see SI 4.1 and 4.2 for detailed analysis). The latter makes rank-3 or closed-walled microstructures impractical for cloaking purposes. Such important insight about the achievable parameter space was not revealed previously, even though the same form of lattice microstructure was adopted in a previous numerical study [33]."

4. I would raise the doubt on novel contribution again after reviewing the whole manuscript. The basic idea is to optimize the microstructure parameters so that they demonstrate the target anisotropic graded thermal conductivities. Then the ideal conductivity tensor required by the thermal device is replaced by the optimized microstructures. Is that correct? Unfortunately, this approach has been well depicted in previous works, though mainly on regular shapes and 2D. In this work, the homogenization method, the inverse design and optimization methods all did not show much novelty (International Journal of Heat and Mass Transfer 169, 120948; International Journal of Heat and Mass Transfer 196, 123149 (6)).

The two studies cited in this comment are about two-dimensional and circular shapes, as shown in the screenshots below, not the three-dimensional and free-form complex geometry that we study, and the latter is far more challenging in many dimensions as articulated in our earlier response, and has not been physically realized thus far. The two studies align well with our argument of novelty and advancement – 2D regular-shape metamaterials have been achieved, but 3D free-form metamaterials have not.





We have cited the two papers in the revised Introduction as shown below.

“Indeed, most realizations of thermal meta-devices thus far remain two-dimensional (2D) mostly with regular shapes (cf., circles) [12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23].”

Reviewer #3 (Remarks to the Author):

This manuscript presents a full design-to-fabrication framework for omnidirectional three-dimensional thermal cloaks with free-form inner and outer boundaries. The authors integrate 3D de-homogenization with a simple, fabrication-friendly three-parameter lattice microstructure to realize the strongly graded and anisotropic conductivity tensors. Their approach leverages transformation thermotics, a robust framework established in 2008 for precisely controlling heat flow. Locally, a surrogate-model-based parameter identification maps desired principal conductivities to bar widths and covers most of the G-closure of two-phase composites. Globally, the method solves for scalar fields whose gradients align with the spatially varying principal directions, enabling an implicit wave-function plus Boolean construction of three mutually orthogonal lattice families that are smooth and naturally connected. Spherical harmonics provide analytic surface representations for complex geometries (e.g., human faces), and a near-transverse-isotropy observation enables robust regularization of ill-behaved eigenvector fields. The authors validate performance through high-resolution finite-element simulations with a relative temperature difference (RTD) metric and through experiments under multiple loading directions. The cloaks maintain straight, equidistant background isotherms and suppress core gradients for a wide range of shapes and material contrasts, outperforming many recent 2D studies while achieving substantially higher geometric complexity. Overall, the manuscript presents a comprehensive methodology with robust, well-validated results, and makes a significant contribution to advancing three-dimensional thermal metamaterials. Before I can recommend acceptance, however, a few issues should be addressed.

We sincerely thank the reviewer for the positive comments and suggestions, and have addressed specific questions point-by-point. The corresponding manuscript revisions are attached in this file in red.

1. The analysis is presented entirely for the steady-state thermal response. Could the authors provide information on the transient behavior of the system? Specifically, what is the characteristic time required for the cloak to reach thermal equilibrium after the boundary conditions are applied? A discussion on how this time scales with the cloak's size and the thermal diffusivity of the constituent materials would be insightful.

   Our experiment observation is that the heat conduction can reach the steady state in about an hour. Quantitatively, the thermal diffusivity of AlSi10Mg is $\beta_A = 45.6\ \mathrm{mm}^2/s$, and that of PDMS is $\beta_B = 0.1\ \mathrm{mm}^2/s$. The two differ by three orders of magnitude. To get an estimate, we instead use an approximation of the composite's average heat capacity $\overline{\rho c}$ using volume averaged specific heat capacity per unit volume and the mean conductivity $\bar{\kappa}$ of the three eigenvalues κ_i, both averaged over the cloak domain. The result are $\overline{\rho c} = 1.464\, J/(cm^3 \cdot K)$ and $\bar{\kappa} = 3.92\, W/(m \cdot K)$.

Using the formula $\bar{\beta} = \frac{\bar{\kappa}}{\overline{\rho c}}$, we obtained the "approximated" $\bar{\beta} = 2.7\ mm^2/s$. The characteristic time of diffusion is defined as $\tau = \frac{L^2}{\beta}$, which scales quadratically with the characteristic length and inversely with diffusivity β. For the pear-apple specimen, the characteristic size is $L = 78\ mm$, which leads to a characteristic time scale of $\tau = 38$ mins. This number is qualitatively consistent to the experimental observation of 50 – 60 mins.

We have added the following discussions on this point in the revised SI 13.3 and mentioned it in the main text.

"In principle, a steady-state thermal cloak cannot conceal an object perfectly from transient thermal detection because transient heat manipulation requires the accurate realization of material density and specific heat capacity, in addition to conductivity [25]. This would pose a greater challenge for engineering compared to the steady-state cloaking."

"Another important aspect about the transient behavior is the estimate of the characteristic time to reach steady state. Here, we use the pear-apple cloak to provide an approximate analysis based on the composite's material properties and show that it qualitatively matches our experimental observation. The specific heat (per unit volume) for AlSi10Mg and PDMS are $\rho_A c_A = 2.46\ \mathrm{J/(cm^3 \cdot K)}$ and $\rho_B c_B = 1.46\ \mathrm{J/(cm^3 \cdot K)}$, respectively. The volume fraction of AlSi10Mg for the pear-apple cloak averaged over the shell domain is 0.004. Using the rule of mixture, the volume-averaged specific heat per unit volume is $\overline{\rho c} = 1.46\ \mathrm{J/(cm^3 \cdot K)}$. For thermal conductivity of the pear-apple cloak, we take the mean of the three eigenvalues and average it over the shell domain, leading to $\bar{\kappa} = 3.92\ \mathrm{W/(m \cdot K)}$. The resulting averaged thermal diffusivity is $\bar{\beta} = 2.7\ \mathrm{mm^2}/s$. For the pear-apple cloak, the characteristic length (height of the cloaking structure) is $L = 78\ \mathrm{mm}$, and hence the characteristic time is $\tau = 38\ \mathrm{mins}$, which qualitatively matches well with our experimental observation of $50 - 60\ \mathrm{mins}$ for entering the steady state. Additionally, the formula of the characteristic time shows a quadratic scaling with characteristic length and inverse scaling with diffusivity."

In the main text's third paragraph of Fabrication and Validation, we have mentioned the investigation:

"…Also, a discussion on the cloaks' transient performance and characteristic time is provided in SI 13.3."

2. Following the previous point, real-world thermal environments are often not perfectly static. How robust is the cloak's performance against dynamic perturbations? For instance, after reaching a steady state, if the external heat source or sink temperature fluctuates within a small range (e.g., sinusoidal or step-wise changes), does the cloaking effect degrade? Please provide a transient

simulation that tracks the Relative Temperature Difference (RTD) under such a perturbation would be a powerful demonstration of the design's practical stability and applicability.

We thank the reviewer for raising this important aspect. For transient cloaking, the transformation theory requires the accurate realization of the density and specific heat capacity in addition to the thermal conductivity, and all three quantities are generally spatially graded. As the density and specific heat are not needed and therefore not considered in the design of the current steady-state cloak, the transient performance of the steady-state cloak is expected to degrade. We fully agree that a transient simulation would provide an informative evaluation on this issue. However, given the large FE mesh size (288 x 288 x 576, needed for high-resolution representation of the structure) and our current computational resources, it may be practically too expensive to perform the transient simulation with many time steps. We would therefore explore it in our future investigation.

We have added the above discussion in the new section of SI 13.3, together with the discussion on the characteristic time, and referred to it in the main text.

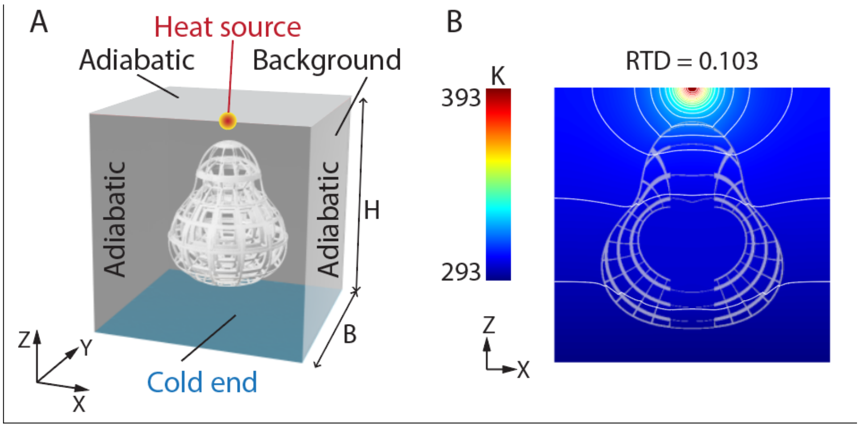
"In principle, a steady-state thermal cloak cannot conceal an object perfectly from transient thermal detection because transient heat manipulation requires the accurate realization of material density and specific heat capacity, in addition to conductivity [25]. This would pose a greater challenge for engineering compared to the steady-state cloaking."

In the main text's third paragraph of Fabrication and Validation, we have mentioned the investigation:

"…Also, a discussion on the cloaks' transient performance and characteristic time is provided in SI 13.3."

3. The current design is optimized for a uniform background temperature gradient. How would the cloak perform if the external thermal environment was fundamentally non-uniform, such as the field generated by a point heat source placed near the cloak? Since the prescribed conductivity tensor is derived based on a uniform field assumption, some performance degradation is expected. A simulation or at least a qualitative discussion on this scenario would help define the operational limits of the proposed design.

   Following the reviewer's suggestion, we have performed an FEA on the pear-apple cloak with a heat source placed near the top of the cloak, as shown in the following figure. For the boundary conditions, only the bottom face of the background domain is Dirichlet with 293 C applied temperature, and the other five faces are adiabatic. We then follow the standard process of computing RTD value based on the temperature fields of the homogeneous background case, the bare case, and the cloak case. The resulting RTD is 0.103, which remains relatively low (for reference, the RTD-X of the uniform background temperature is 0.079), demonstrating an overall satisfactory cloaking performance under non-uniform background temperature with heat sources.



We have added a paragraph discussing this point in SI 10.3, as attached below.

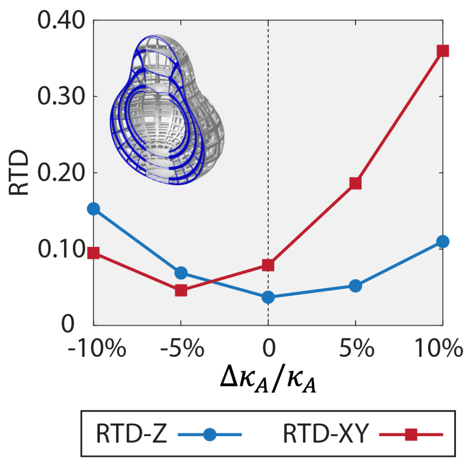
"The 3D cloak also performs well with the presence of a point heat source in the background. We demonstrate this by FEA with a concentrated heat source placed near the top of the pear-apple cloak, as shown in Figure 9B. For boundary conditions, the bottom face of the domain is set to a constant temperature, while the other five faces are adiabatic. The heat generated at the top will travel through the domain and reach the cold end at the bottom. The resulting temperature distribution of the X-Z mid-plane is shown in Figure 9C, overlaid with the 3D cloak. The RTD value measuring the relative difference between the temperature and that of the homogeneous background is 0.103, an overall satisfactory performance. This demonstrates the consistent cloaking performance under a non-uniform background temperature caused by a heat source."

The conclusion is mentioned in the revised main text in the paragraph before the Fabrication and Validation section as follows.

"…We note that the cloaking performance is insensitive to the core material (the cloaked object, see SI 10.1), the background material (see SI 10.2), and the presence of a heat source in the background (see SI 10.3). However, it is influenced by the fluctuation of material properties (see investigation in see SI 10.4)…."

4. The authors are commended for advancing free-form cloaking, which moves the field closer to real-world implementation. In practical scenarios, material properties can deviate from their designed values due to manufacturing inconsistencies, operational wear, or material aging. Could the authors perform a sensitivity analysis to quantify the impact of such perturbations on the cloak's performance? For example, how does the RTD change if the thermal conductivities of the AlSi10Mg and PDMS constituents vary randomly by ±5% or ±10% from their nominal values?

Following the reviewer's suggestion, we have conducted FEA on the pear-apple cloak by varying the conductivity of Material A (AlSi10Mg) κ_A by ±5% and ±10%, and the results are shown in the following figure. For Material B (PDMS), as its conductivity is three-orders of magnitude smaller than Material A's, its variation within 10% should not cause great changes in RTD. As shown in the figure, the RTD-Z value is relatively insensitive to the perturbation of κ_A, with all values lower than 0.16. By contrast, the RTD-XY is more sensitive to the increase of κ_A, where the RTD-XY takes a spike to 0.36 when κ_A rises by 10%. However, the drop in κ_A does not cause a strong deterioration of RTD-XY. The RTD's sensitivity to material property perturbation is generally case-dependent.



We have added a discussion on this aspect in the revised SI 10.4 as attached below.

"In practice, material properties can deviate from their designed values due to, for example, manufacturing inconsistencies or aging. In the current context of thermal cloak, the conductivities of AlSi10Mg and PDMS can differ from their nominal values. Here, we investigate the influence of such fluctuation on the cloaking performance (RTD values) under ±5% and ±10% variation in κ_A. For Material B (PDMS), as its κ_B is three orders of magnitude smaller than κ_A, its limited variation should not cause a huge change in RTD values.

The RTD values of the pear-apple cloak under the perturbation of κ_A are shown in Figure 9A. The RTD-Z is relatively insensitive to material's fluctuation, and all values within 10% of property change are below 0.16. In contrast, the RTD-XY values are more sensitive when κ_A increases, reaching a value of 0.36 at 10% increase. The sensitivity to material property variation, however, is generally case- and design-dependent."

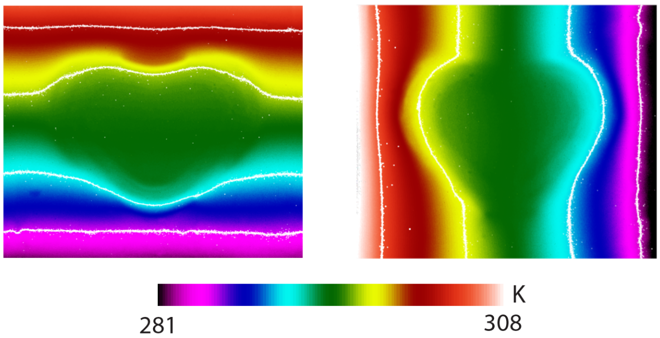
The conclusion is mentioned in the revised main text in the paragraph before the Fabrication and Validation section as follows.

"…We note that the cloaking performance is insensitive to the core material (the cloaked object, see SI 10.1), the background material (see SI 10.2), and the presence of a heat source in the background (see SI 10.3). However, it is influenced by the fluctuation of material properties (see investigation in see SI 10.4)….”

5. The analysis assumes perfect thermal contact at the interface between the AlSi10Mg lattice and the PDMS matrix. In a real composite, a non-zero interfacial thermal resistance will exist. Could the authors provide an estimation of the potential impact of this resistance on the cloak’s performance? A brief parametric study showing the change in RTD as a function of a plausible range of interfacial resistance values would significantly strengthen the experimental claims.

   It appears that the influence of the interfacial thermal resistance on the overall cloaking performance in our case is relatively weak, as we have not observed sharp changes of temperature across the aluminum and PDMS parts – a typical sign of strong interfacial resistance. For example, the figure below shows the front-face temperature distribution of the heart-shaped cloak (with the overlayed structure removed). The temperature distribution across the aluminum and PDMS parts are by-and-large smooth and gradual. Also, the background’s isotherms are largely straight and uniform, suggesting a good cloaking effect. These observations seem to suggest that the impact of interfacial resistance may be limited.

   We fully agree on the value of a numerical study on this issue but deem it a future investigation. It would require an extremely fine and unstructured FE mesh for the interfacial layers that are beyond our current computational capacity.



   We have added a discussion on this important aspect in SI 13.2 as follows.

   “Interfacial thermal resistance between the aluminum and PDMS parts may arise, but its impact on the overall cloaking performance appears to be limited as the experimental temperature distribution across the two materials is, by and large, smooth and gradual (Figure 11 A), without the sharp changes that typically signify strong interfacial resistance. This observation, however, may not be generalizable to other materials and setups. Numerical and experimental investigations into the influence of interfacial resistance on the performance of thermal meta-devices would be a valuable future investigation.”

In the main text's third paragraph of Fabrication and Validation, we have mentioned the investigation:

"…We note that the choice of the base materials imposes certain practical requirements on the application conditions, such as the operational temperature at which the material properties are stable and the potential influence of interfacial thermal resistance (see SI 13.1 and 13.2 for investigation)…."

6. To better situate this contribution within the developing thermal metamaterials, I suggest that the authors add a statement to a discussion section. Specifically, they should clarify how their work exemplifies and advances the "free-form" design paradigm, which was recently conceptualized in works such as Xu et al., Nature Computational Science, 4(7):532-541, 2024. The authors are to be commended for the complexity and novelty of the shapes demonstrated. While much of the prior research in transformation thermotics and metamaterials has focused on cloaking geometrically regular objects (e.g., circles, polygons), the pear and human-face shapes presented in this work are an excellent realization of a truly free-form design. This represents a significant step forward, moving the field of thermal cloaking from idealized geometries toward practical applications where objects have arbitrary and complex contours.

We appreciate the reviewer's compliment. We have added a discussion session to the end of the main text to better summarize and discuss our innovations and impacts, as shown in the following.

"This study demonstrates a precise, efficient, and practical design-fabrication strategy for realizing omnidirectional, arbitrary-shaped 3D thermal meta-devices predicted by transformation theory. This is made possible by integrated innovations from multiple spheres, including 1) the discovery of special spectral properties of the transformed 3D conductivity that significantly accelerates the subsequent design process; 2) the proposed geometrically simple 3D lattice microstructure with revealed large effective property space; 3) a new 3D de-homogenization technique featuring multi-step Boolean operations tailored to the 3D lattice; 4) the integration of transformation thermotics with spherical harmonics equipped with a proposed transverse isotropy regularization.

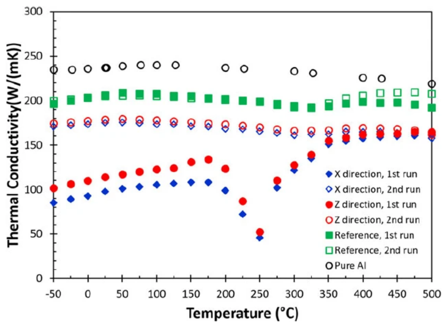
The combined innovations enable the creation of 3D thermal meta-device structures that are locally concise, naturally well-connected, capable of adapting to highly complex domains, and practically fabricable. Regardless of the geometry, the 3D thermal cloaks demonstrate great performance in concealing objects under multi-directional thermal detection, as evidenced by the small RTD index. With metal 3D printing, we accurately fabricate the 3D thermal cloak and successfully reproduce the omnidirectional cloaking effect in the experiment.

The findings provide a competitive and general solution to the long-standing challenge of accurately realizing 3D graded and anisotropic material properties. They also move the field of thermal metamaterial from idealized 2D geometries toward practical applications, where objects have arbitrary and complex 3D geometries. The developed methodology is general and transformable, readily extensible to other 3D thermal and conduction-dominated meta-devices across various disciplines."

7. The current study masterfully addresses the thermal performance of the cloak, assuming stable material properties. However, for potential applications in high-temperature environments (e.g., aerospace, waste heat management), the thermo-mechanical integrity of the structure becomes a critical consideration. The mechanical properties of both the AlSi10Mg lattice and the PDMS matrix are known to be temperature-dependent. Could the authors please discuss the anticipated operational temperature limits of their proposed design?

   We thank the reviewer for raising this fruitful point. For PDMS, the chemically stable temperature is around 200 °C. For AlSi10Mg, the restriction is from the thermal perspective to retain stable thermal conductivity. As shown in the plot below from *Journal of Materials Research, 22(23): 4040-4052, 2018*, the conductivity of 3D-printed AlSi10Mg remains relatively stable when the temperature is below 150 °C, hence 150 °C may be an appropriate upper limit of operational temperature.

   We have added a description (attached below) on this point to SI 13.1 of the revised manuscript.



   "In general, materials' properties (such as thermal conductivity, mechanical stiffness, and chemical stability) are temperature-dependent, which may impact the cloak's performance under different operational temperatures. For our realization with AlSi10Mg and PDMS, the thermal conductivity of AlSi10Mg remains relatively stable when the temperature is below 150 °C [24]. For PDMS, as its conductivity is about 0.1% of the conductivity of AlSi10Mg, the variation should not greatly impact the overall cloaking performance. The chemically stable temperature for PDMS is below 200 C. Hence, the operational temperature for the current realization of 3D cloak shall be lower than 150 °C. An operational temperature higher than this value may require a change of the base materials, to which the proposed design method is also directly applicable."

   In the main text's third paragraph of Fabrication and Validation, we have mentioned the investigation:

   "…We note that the choice of the base materials imposes certain practical requirements on the application conditions, such as the operational temperature at which the material properties are stable and the potential influence of interfacial thermal resistance (see SI 13.1 and 13.2 for investigation)….”

8. It is anticipated that additional relevant references, including review articles and monographs, will be incorporated into the reference list to benefit readers. Additionally, a minor formatting issue has been identified in the manuscript. Specifically, units should be presented in their standard form, and a space must always be inserted between a numerical value and its corresponding unit.

   The formatting of the units is corrected as suggested. We have added the following references in the revised manuscript (including SI).

   - Qingxiang Ji, Xueyan Chen, Jun Liang, Vincent Laude, Sébastien Guenneau, Guodong Fang, and Muamer Kadic. Designing thermal energy harvesting devices with natural materials through optimized microstructures. International Journal of Heat and Mass Transfer, 169:120948, 2021.
   - Qingxiang Ji, Xueyan Chen, Jun Liang, Guodong Fang, Vincent Laude, Thiwanka Arepolage, Sébastien Euphrasie, Julio Andrés Iglesias Martínez, Sébastien Guenneau, and Muamer Kadic. Deep learning based design of thermal metadevices. International Journal of Heat and Mass Transfer, 196:123149 (6), November 2022.
   - Ting-Hua Li, Dong-Lai Zhu, Fu-Chun Mao, Ming Huang, Jing-Jing Yang, and Shou-Bo Li. Design of diamond-shaped transient thermal cloaks with homogeneous isotropic materials. Frontiers of Physics, 11(5):110503, Apr 2016.
   - Qi Li and Jeffrey S. Vipperman. Non-singular three-dimensional arbitrarily shaped acoustic cloaks composed of homogeneous parts. Journal of Applied Physics, 124(3):035103, 07 2018.330
   - Qingxiang Ji, Xueyan Chen, Jun Liang, Vincent Laude, Sébastien Guenneau, Guodong Fang, and Muamer Kadic. Non-singular homogeneous polyhedral heat cloak and its realization. ES Energy and Environment, 7:29–39, 2020.
   - Pin Yang, Lisa A. Deibler, Donald R. Bradley, Daniel K. Stefan, and Jay D. Carroll. Microstructure evolution and thermal properties of an additively manufactured, solution treatable alsi10mg part. Journal of Materials Research, 33(23):4040–4052, Dec 2018.
   - Sebastien Guenneau, Claude Amra, and Denis Veynante. Transformation thermodynamics: cloaking and concentrating heat flux. Opt. Express, 20(7):8207–8218, Mar 2012.
   - Liujun Xu, Pengfei Zhuang, Fubao Yang, Shuihua Yang, Chengmeng Wang, Gaole Dai, Jiping Huang, and Cheng-Wei Qiu. Heat diffusion invariant. Phys. Rev. Lett., 135:067103, Aug 2025.

The authors are most grateful for the editor's and reviewers' careful reading and thoughtful comments and suggestions for our manuscript titled "Free-form thermal cloaks in three dimensions", by Weichen Li, Yibo Wang, Ole Sigmund, Xiaojia Shelly Zhang. We have revised the main manuscript and Supplementary Information according to all the comments. The point-to-point response is highlighted in **blue**, and the corresponding changes in the revised manuscript and Supplementary Information are highlighted in **red**. Below we address each comment in detail.

Reviewer #1 (Remarks to the Author):

Although several questions have been clarified, many points still remain unclear, and it is necessary to provide responses to the comments below.

1. In the reply to Comment 4 of Reviewer #1, the authors provide a table in the response letter to compare their study with previous studies. This table should be included in the manuscript to highlight the novelty of the presented study.

We thank the reviewer's suggestion. As shown below, we have included the table in the SI Sec. 8 of the revised manuscript, where we compare various methods for thermal metamaterial design.

"Table 1 summarizes the key features of these methods, which are also discussed in more detail as follows."

Table 1: Summary of three strategies for the design of free-form omnidirectional thermal metamaterials in 2D and 3D spaces

Metamaterial design strategy	**Divide and conquer + TO microstructure** (e.g., Nat. Commun., 12(1):7228, 2021)	**Divide and conquer + AI microstructure** (e.g., Advanced Materials, 35(33):2302387, 2023)	**3D de-homogenization + simple 3D microstructure** (This study)
Dimension realized	2D	2D	3D
Direction dependence	Omnidirectional	Omnidirectional	Omnidirectional
Microstructure inverse design cost in 3D case	Not demonstrated in 3D, but expectedly very high cost as each unit cell requires a 3D TO process with numerical homogenization (quantitative computational cost not reported)	Not demonstrated in 3D, but presumably low-cost after potentially expensive ML training (quantitative computational cost not reported)	Low cost, thanks to geometric simplicity and surrogate model (¡1 sec. per microstructure)
Global structure generation method	Unit cell assembly + post-processing	ML-based unit cell assembly	3D de-homogenization
Global 3D connectivity	Not demonstrated in 3D, but based on the 2D version, heavy post-processing should be required	Not demonstrated in 3D, connectivity guaranteed in 2D	Naturally guaranteed without post-processing
Global structure fabricability	Not demonstrated in 3D, but the high complexity of 3D TO-microstructure would be challenging to fabricate	Not demonstrated in 3D, but the high complexity of 3D AI-microstructure would be challenging to fabricate	Practically fabricable as demonstrated
Cloaking performance in RTD	Not demonstrated in 3D nor reported in 2D	Not demonstrated in 3D, the 2D reported values of free-form geometries are 0.13 - 0.39	RTD in 3D with similar geometric complexity is 0.03 - 0.15

2. In the above table in the response letter, the authors claim that the presented method provides a "global optimum (within the achievable range)." How did the authors verify that the obtained structures correspond to a "global optimum"? The authors need to explain the method used to demonstrate the global optimality of the presented optimized structures?

We thank the reviewer's insightful comment. There are three potential error sources that may perturb the microstructure from attaining the exact theoretical homogenized properties. The first is the practically finite-periodicity structures instead of the idealized infinite periodicity assumed in homogenization theory. The second source is the FE discretization error in numerical homogenization. The third is that the target properties required by transformation thermotics are beyond the achievable region of the microstructure. The first two sources are generally present for any numerical methods considering microstructures. For the third source, there exists a thin-layer region near the inner core that requires close-to-zero conductivity in the radial direction, which is lower than the insulating base material's κ_B (in our case, $\kappa_B = 0.16\ \mathrm{W/(m \cdot K)}$), implying it is outside the theoretical bounds of the G-closure regardless of the microstructure's form. Hence, the third error source is also general for all methods.

However, in the case that the target conductivity is within the achievable range of a microstructure (i.e. no error in the third source) and in the case the finite periodicity and FE discretization error is negligible, our parameter identification can obtain the global optimum numerically (also unique except for the maximum isotropic point of $\boldsymbol{\kappa} = \kappa_A \boldsymbol{I}$). This is because our three-parameter mapping $\boldsymbol{b} \to \boldsymbol{\kappa}$ is bijective and invertible for $b_i \in [0,1)$ (excluding $b_i = 1$ that matches $\boldsymbol{\kappa} = \kappa_A \boldsymbol{I}$). It is also because the domain and co-domain of the mapping are both compact and simply connected, and the determinant of $\frac{\partial \boldsymbol{\kappa}}{\partial \boldsymbol{b}}$ is numerically verified to be strictly greater than 0. This means the existence of an inverse map $\boldsymbol{\kappa} \to \boldsymbol{b}$, and hence, for any reachable target $\boldsymbol{\kappa}$ (except $\boldsymbol{\kappa} = \kappa_A \boldsymbol{I}$), there is a unique corresponding $\boldsymbol{b}$. This is not the case for topology optimization.

Therefore, our "global optimum" was referring to the microstructure's unique attainment of a reachable $\boldsymbol{\kappa}$, not counting the general numerical error sources of finite-periodicity and FE discretization error. To avoid confusion, we have removed the claim in Table 1 in the first comment (also added to SI Sec. 8).

3. Doesn't the computational cost of mapping between physical property data and microstructure data largely depend on how detailed the acquisition of the physical property data and the microstructure data is?While these mapping data may be reusable, this computational cost cannot be ignored.

The computational cost of building the surrogate model off-line is approximately 32 hours in our case. However, we would argue that it would be misleading and indeed incorrect to count it as part of the design cost of a thermal cloak because the cost is design-independent. It is constructed only once and reused for any number of new designs. This is to be differentiated from the free-form inverse design approach (such as topology optimization), where the creation of each new design requires on-the-fly numerical homogenization involving hundreds of solves for the state equation. These two approaches are clearly and fundamentally different in terms of whether numerical homogenization is involved for a new design, and our current definition of design cost reveals such a difference objectively and distinguishably. Hence, the cost of surrogate model construction is not included as part of the design cost but is reported independently.

We have added the cost of building the surrogate model in the revised SI Sec. 4.1 as shown below.

"The parameter sweep is performed in four parallel groups on a desktop workstation and takes approximately 32 hours. The off-line surrogate model needs to be constructed only once and is reused for creating any new 3D thermal cloak."

4. Related to the above comment, it is necessary to investigate how the resolution of the data mapping affects the optimization results. Wouldn't these factors strongly influence the reproducibility of the results?

We thank the reviewer's comment on the discretization resolution. We did carry out investigations on this subject, where we tried resolutions of 16×16×16, 32×32×32, and 64×64×64 in building the surrogate model and then used them for the parameter identification. Our observation is that the results using the latter two resolutions show negligible difference, and hence the 32×32×32 is chosen for better efficiency.

To convey the above idea, we have added the following comment in SI Sec. 4.1 as follows.

"For our implementation, we used a discretization of 32 intervals (33 points) for the parameter sweep of b_i. Our investigation on discretization resolution shows that the chosen value is a good balance between accuracy and efficiency for the proposed 3D microstructure."

Reviewer #2 (Remarks to the Author):

I am fine with the implementations. It can be published.

Reviewer #3 (Remarks to the Author):

Three-dimensional thermal cloaks of arbitrary shapes hold immense application value in the infrared thermal protection of underground bunkers. This manuscript presents a comprehensive methodology accompanied by robust and well-validated results, making a significant contribution to the advancement of three-dimensional thermal cloaks, which are a representative example of metamaterials. The author has satisfactorily addressed all my queries, and I am more than willing to recommend this paper for publication in Nature Communications.