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Theoretical study in dual-channel quasi bound-states in the continuum in YaBa₂Cu₃O₇ ceramic split-ring resonator metasurface and multi-functional responsive sensing

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ABSTRACT

In recent years, quasi-bound-states in the continuum (q-BIC) have been widely studied, and mechanisms for exciting q-BIC have been continuously proposed. In the research of q-BIC, symmetric-protecting q-BIC is an important branch, and as a classic metasurface design scheme, a split-resonant ring (SRR) has been found to excite q-BIC. A dual-channel q-BIC design is proposed based on the symmetry-breaking property of YaBa₂Cu₃O₇ ceramic SRR metasurface. Two asymmetry parameters are introduced into YaBa₂Cu₃O₇ ceramic SRR metasurface, which can excite q-BIC channels at two frequency positions, respectively. This characteristic is utilized to analyze sample thickness and detect refractive index separately at two q-BIC channels. The q-BIC channel 1 is used as a responsive thickness sensor to detect the thickness of the sample layer. The q-BIC channel 2 realizes the function of refractive index detection. Herein, a method is provided for exciting dual-channel q-BIC and utilizing the high quality factor of q-BIC to achieve multi-functional sensing. It has enormous potential value in biomedical and environmental monitoring fields.

1. Introduction

A metasurface is a metamaterial composed of periodically arranged subwavelength structures [1]. The electromagnetic (EM) properties of metasurfaces are mainly determined by their shape, size, and spatial distribution [2]. In recent years, the significant regulatory effect of metasurfaces on EM properties has attracted widespread attention from researchers [3-6]. Among them, metasurfaces are used to form sound manipulation of EM waves, such as coherent perfect absorption [7], local resonances [8], and Tamm states [9]. Metasurface sensors are important in metasurface research [10,11], and metasurface resonant structures have significant value in sensor design [12]. The resonator will generate strong field localization effects near the resonant frequency, and the tested substance will experience resonance effects with EM waves [13,14]. The quality factor (QF) is an essential indicator for measuring the performance of sensors [15,16], a high QF means stronger interaction between waves and matter [17,18]. To obtain a high QF, bound-states in the continuum (BIC) [19-22] are introduced for the scheme of metasurfaces. In the conventional view, the resonant states that exist in the radiation continuous domain radiate energy outward [22], and perfect bound states only exist outside the radiation continuous state [23]. The emergence of BIC has broken this bottleneck and formed a perfect bound state in a continuous domain that does not radiate any energy [23]. Since Von *et al.* [24] first proposed the concept of BIC in 1929, its mathematical model and engineering applications have been widely studied [25–27]. Common types of BIC include Fabry–Pérot BIC e [28], symmetric-protecting typed BIC [29], resonant typed BIC [30], etc. In 2018, Kirrl *et al.* [31] proposed an asymmetric metasurface and conducted rigorous theoretical verification. Several typical symmetric-protecting typed BICs have been summarized. In recent years, there has been an increasing amount of research on BIC, and the theoretical explanation has been basically complete [32,33]. However, some remarkable optical phenomena related to quasi-BIC (q-BIC) still need to be explored [31].

Split-ring resonator (SRR) is often used for designing metasurfaces, it has an extremely wide range of applications [34], such as negative refractive index [35], asymmetric control [36], EM induced transparency [37], etc. Shelby *et al.* [38] used SRR arrays and metal wires to

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fabricate the first left-handed material. In 2023, Guo *et al.* [39] designed a high *QF* SRR metasurface that helps enhance sensing performance. However, improving *QF* has always been an urgent issue for SRR, and q-BIC has to be introduced for SRR design. In 2019, Cong *et al.* [40] utilized SRR to achieve symmetric-protecting q-BIC, achieving an extremely high *QF*. The current BIC design mainly focuses on singlechannel BIC, which is difficult to complete the design of multifunctional optical devices [31]. Combining SRR for BIC design is an effective method to improve sensing performance [41]. However, the proposal of multitasking sensing scenarios requires the realization of multi-channel and multi-asymmetric q-BIC.

The frequency range corresponding to terahertz (THz) waves is 0.1-10 THz [42], with strong penetrability and sensitivity to weak resonance. THz spectroscopy records amplitude and phase information, making it easy to extract the dielectric properties of the analyte. The EM waves of THz can achieve unique spectral fingerprinting and substance identification [43]. Many biochemical molecules undergo molecular vibrations in the THz band, so these biochemical molecules can be detected in the THz band [44,45]. Gases have harmless rotational and vibrational characteristics in the THz band. THz waves can penetrate biological tissues without ionization, which is of great significance in non-invasive detection [44–46]. The detection of human exhaled gas can effectively reveal the diseases that may exist in the human body, such as diabetes, cancer, etc [47]. Therefore, the gas sensors are important in the sensor field, and designing suitable gas sensors has significant value in gas quality detection [48], human health monitoring, and other aspects. By using BIC to increase the QF of sensors in the THz band, the performance of sensors can be improved, which is used for biological detection and air quality supervision. However, the current THz BIC design mainly relies on the medium with high reflection characteristics such as metal, which is far less QF than the BIC in the optical band due to the existence of loss.

Herein, the lossless properties of YaBa₂Cu₃O₇ ceramic material is utilized, a YaBa₂Cu₃O₇ ceramic SRR metasurface (YCSM) with dualchannel q-BIC is designed. Two asymmetry parameters α and X (see Fig. 1(c)) are introduced to excite the dual-channel q-BIC. Dual-channel q-BICs are excited at $f_1 = 1.223$ THz and $f_2 = 2.455$ THz, where α corresponds to the q-BIC at f_1 and X corresponds to the q-BIC at f_2 . The q-BIC has the characteristic of infinite high QF [40]. The problem of low QF in traditional THz BIC design is overcome, and the function of multifunctional responsive sensing is realized. In biological measurement, virus detection and gas components detection are extremely important research topics [45,48]. As such responsive thickness sensor (RTS) and responsive refractive index sensor (RRIS) are raised based on YCSM. The high *QF* of the two BIC channels in this article can be used for designing RTS and RRIS. The BIC at f_1 achieves thickness detection, while the BIC at f_2 forms refractive index detection. It has potential applications in biological detection, disease treatment, environmental monitoring, and other fields.

2. Configuration of YCSM and excited dual-channel q-BIC

2.1. Configuration

As shown in Fig. 1(a)–(c), a YCSM is given. The array structure of YCSM is shown in Fig. 1(a), while the schematic diagram of a single YCSM is shown in Fig. 1(b). The YCSM consists of a substrate and four SRRs. In the initial configuration, the dimensions and positions relative to the center of the YCSM of the four SRRs are exactly the same, they are defined as S1, S2, S3, and S4. A beam of THz y-polarized EM waves (the electric field vector vibrates along the +y-axis direction and the magnetic field vibrates along the +x-axis) enters the YCSM from the +z-direction [2]. The plane figure of the YCSM +z-direction is shown in Fig. 1 (c), from which the geometric parameters of YCSM can be observed. To study the q-BIC effect, it is necessary to break the symmetry breaking property of YCSM. Two asymmetry parameters are introduced to excite q-BIC. $\alpha = 2w/L$ is the axial asymmetry parameter, representing the movement of S_1 and S_2 in the y-direction, details can be seen in Fig. 2(a). Another asymmetry parameter is the rotation angle of S₃ and S₄ towards the center, where S_3 rotates clockwise by X° and S_4 rotates counterclockwise by X° , as shown in Fig. 3(a). Two asymmetry parameters excite q-BIC at two frequency points respectively. The substrate material is porous silicon (PSi) and $n_{PSi} = 1.45$ [49], and the SRRs in YCSM are composed of YaBa₂Cu₃O₇ ceramic [50], which exhibits reflective properties in the THz band, it is used for the excitement of q-BICs in this paper.

Section 3 of Supplementary Material provides a detailed analysis of multipole analysis, from which the intensities of electric dipoles (ED),



Fig. 1. When EM waves enter with *y*-polarized, (a) schematic diagram of array structure of YCSM, (b) main view of a single YCSM, a YCSM consists of a layer of substrate and four SRRs, where $H = 30 \mu$ m, $t = 10 \mu$ m, and (c) the top view of YCSM, where the four SRRs are named S₁, S₂, S₃, and S₄, and for a YCSM, the total length and broadband are $P_x = P_y = 100 \mu$ m, for two separate SRRs, as S₃ and S₄, the distance is $L = 50 \mu$ m, the radius of the outer ring of each separate SRR is $r_2 = 18 \mu$ m, the radius of the inner ring is $r_1 = 15 \mu$ m, and the width of the gap is $g = 6 \mu$ m, at 0.5–2.5 THz, the YCSM exhibits (d) reflection spectral lines, (e) multipole analysis.



Fig. 2. (a) Top view when YCSM has asymmetry parameter α ; (b) The resulting curves at 1.225 THz, with α ranging from -0.2-0.2, (c) the fitting curve between QF and α , (d) Multipole analysis with asymmetry parameter α , (e) current intensities distribution, and (f) electric field intensities distribution at 1.225 THz.



Fig. 3. (a) Top view of the YCSM with asymmetry parameter *X*, (b) The influence of reflection spectral lines when *X* changes, where $X \neq 0^{\circ}$ represents q-BIC, and (c) The linear relationship between *QF* and *X*, (d) multipole analysis with asymmetry parameter *X*, (e) current intensities distribution and (f) electric field intensities distribution, and (g) magnetic field intensities distribution at 2.476 THz.

magnetic dipoles (MD), and tropical dipoles (TD) can be obtained [51–54]. The *y*-polarized EM waves spectrum of YCSM in the range of 0.5–2.5 THz is shown in Fig. 1(d), with a resonant peak at 1.235 THz. The multipole scattering power near 1.235 THz is calculated to determine the excitement cause of this resonance peak. As shown in Fig. 1(e), the scattering power of the ED is highest at this time, indicating that the resonance peak here is contributed by the ED. In the design of

metasurface sensors, such peaks can not meet the requirements of high QF. To excite the q-BIC phenomenon in YCSM, asymmetry parameters α and X are introduced. In this section, the main reasons for the generation of q-BICs are analyzed, therefore perfect electrical conductor [6] is used to replace YaBa₂Cu₃O₇ ceramic to simulate the almost total reflection of the substrate and conduct multipole analysis.

2.2. Introduction of q-BIC

The mode of q-BIC can perfectly confine energy within a limited area [31]. In theory, when q-BIC occurs, it corresponds to an infinite *QF*, which have theoretically explained by Liang *et al.* [32]. The important role of q-BIC effect in improving sensing performance is mainly reflected in its high *QF* property [33]. When introducing asymmetry parameters in YCSM, q-BIC is excited, which has a finite high *QF* [32]. Asymmetry parameter α is introduced into YCSM, can be seen from Fig. 2(a). The intuitive representation of α can be seen from Fig. 2(a). When $\alpha = 0$, there is only one resonant peak formed by an ED in the spectrum.

As asymmetry parameter α changes, it is necessary to calculate the *QF*. In symmetric-protecting q-BIC, the *QF* should satisfy the *QF* $\propto \alpha^{-2}$ relationship, as shown in Fig. 2(c) [31]. The fano fitting method [53] is used to calculate the *QF* of q-BIC, when the *QF* is high enough (*QF* > 100) [53], Fano fitting can be approximately solved using the full width at half maxima method [53]. The calculation results of *QF* are reflected in Fig. 2(c), it is found that a approximately linear relationship is maintained between *QF* and α^{-2} , which satisfies the relationship of symmetric-protecting typed q-BIC [31].

To further illustrate the functional mechanism in YCSM, the method of multipole analysis [53] is adopted. Analyze the multipole categories at this time by calculating the scattering power when $\alpha = 0.15$. From Fig. 2(d), it can be seen that when symmetry is broken, the contributions of ED and TD are relatively strong, while the contributions of other multipole modes are weaker. In Fig. 2(d), it can be seen that the electric field energy is localized at the gaps of S₃ and S₄ in Fig. 2(e). The magnetic field energy intensities are mainly distributed at the split region, as shown in Fig. 2(f). This indicates that the q-BIC at 1.225 THz is generated by ED.

The second asymmetry parameter is defined as *X*, which is the rotation angle of S₁ and S₂ relative to the dashed line. The intuitive definition of *X* is reflected in Fig. 3(a), where the dashed line represents the base line. When $X = 0^{\circ}$, the peak is excited, forming a symmetry-protecting typed q-BIC [32]. When $X = 0^{\circ}$, the reflection spectrum is extremely low and smooth between 2.45–2.5 THz. During the process of *X* increasing, the symmetry breaking property is broken, and leaks into the radiation channel, thus forming q-BIC resonance [32]. The situation where *X* increases from 1° to 5° is shown in Fig. 3(b), and exhibits q-BIC characteristics at case of $X \neq 0^{\circ}$. As *X* increases, the *QF* continuously decreases. The resulting curves are shown in Fig. 3(c), where *QF* and *X* exhibit a quadratic relationship, satisfying the criterion for q-BIC [31].

In this case, the MD is often the main contributor to the EM field, especially in areas far from the current source, where the contribution of the MD field usually dominates, the characteristics of the MD can be intuitively seen from the current graph. However, when conducting more accurate multipole analysis, higher order multipole terms need to be considered. Therefore, the mechanism of YCSM with asymmetry parameter X, the EM distributions of far-field and near-field situations are analyzed. The multipole analysis on the presence of asymmetry parameter X is conducted. In Fig. 3(d), the scattering power of each multipole at $X = 5^{\circ}$ is investigated. The results indicate that TD dominates in multipoles when asymmetry parameter X exists. TD can effectively reduce radiation loss and achieve good suppression effect at 2.476 THz, realizing q-BIC mode [31], as shown in Fig. 3(b). To further illustrate the mechanism of YCSM with asymmetry parameter X, the EM distributions of far-field and near-field are analyzed in Fig. 3(d)-(g). The direction of current flow at 2.476 THz in the YCSM is shown in Fig. 3(e). The blue arrows indicate the direction of current flow, forming opposite currents around SRR, reflecting the properties of MD [51]. With the right-hand screw rule [53], it can be concluded that the direction is pointing in the -z-direction. Analysis of the ED, MD, TD, and quadrupole results in the +y-direction (seen in Fig. 1(b) and Fig. 3(e), respectively) indicate that the TD contributes the most at this time. In current diagram observation from Fig. 3(3), only the first-order approximation, namely the MD, is usually focused on. In Fig. 3(f) the energy map of the

electric field at 2.476 THz of q-BIC is shown. The results indicate that the energy of the electric field is localized on the upper and lower sides of the SRRs. The distribution of magnetic field energy is discussed in Fig. 3 (g), with the magnetic field energy field intensities distributed at the SRR and its symmetrical position. The EM field and far-field analysis well demonstrate that the q-BIC here is excited by TD.

The results are calculated when the SRR material is YaBa₂Cu₃O₇ ceramic as shown in Fig. 4(a)–(c). From Fig. 4(a), it can be seen that TD dominates in the multipole effect. In Fig. 4(b) and (c), the YCSM achieved two q-BICs at positions $f_1 = 1.223$ THz and $f_2 = 2.455$ THz, respectively. For the refractive index of YaBa₂Cu₃O₇ ceramic materials, the dielectric function is described using the two-fluid model and London local electrodynamics [55]. In instances where the temperature remains below the critical temperature, the behavior of the superconductor can be approximated as lossless [56]. Consequently, the dielectric function model is represented as [50]:

$$\varepsilon_Y = 1 - \frac{1}{\omega^2 \mu_0 \varepsilon_0 \lambda_L^2} \tag{1}$$

where $\lambda_{\rm L}$ is the temperature-dependent London penetration length, which can be represented as [50],

$$\lambda_L = \frac{\lambda_L(o)}{\sqrt{1 - \left(\frac{T_0}{T_C}\right)^{P_0}}}$$
(2)

where $\lambda_L(o) = 200$ nm is the London penetration length at ambient temperature $T_0 = 55$ K, $P_0 = 4$, and $T_C = 92$ K is the superconducting critical temperature [55]. The reflection spectrum of YCSM is given in Fig. 4 (a), and the f_1 and f_2 marked in Fig. 4(a) indicate that two q-BICs will be excited at these two positions. When asymmetry parameters are introduced, q-BICs are excited, as can be seen from Fig. 4(b) and (c). This effect can form sharp reflection peaks with high QF, which can be used in multi-functional responsive sensing.

3. q-BIC channels applied in RTS and RRIS

In the evaluation system of optical sensors [57], figure of merit (*FOM*), detection limit (*DL*), sensitivity (*S*), and *QF* are common evaluation indicators. The calculation formulas for *S*, *DL*, and *FOM* are as follows [57]:

$$S = \frac{\Delta f}{\Delta r}$$
(3)

$$FOM = \frac{S}{FWHM}$$
(4)

$$DL = \frac{f}{20 \cdot S \cdot Q} \tag{5}$$

The schematic diagram of RTS unit cell is shown is Fig. 5(a), Teflon is the carrier medium [44], the dielectric properties of a common sample is used to model the sample to be detected [44]. The q-BIC occurs at f_1 = 1.223 THz (α = 0) is defined as q-BIC channel 1. When the asymmetry parameter α is introduced, the q-BIC channel 1 is excited. Due to its high *QF*, it can be used for responsive sensors. When conducting THz sample thickness detection, the schematic diagrams of RTS can be seen in Fig. 5 (b)–(e). Teflon [58] is used as a carrier for the analyte and placed in a SRR, while sample is prevented from being present on Teflon. The thickness of Teflon is $d_{\text{Teflon}} = 0.5 \,\mu\text{m}$, and the refractive index is n_{Teflon} = 1.46 [58]. The dielectric properties of sample can be described by Drude-Lorentz model [58]:

$$\varepsilon_r = \varepsilon_{\infty} + \sum_{p=1}^{\infty} \frac{\Delta \varepsilon_p \omega_p^2}{\omega_p^2 - \omega^2 - j\gamma\omega}$$
(6)



Fig. 4. (a) The reflectance spectrum of YCSM in the range of 0.5–2.5 THz; when asymmetric parameter (b) α is introduced at f_1 and (c) X is introduced at f_2 .



Fig. 5. (a) Schematic diagram of RTS unit cell, (b) Peak position of q-BIC varies with d; (c) linear fitting curve of RTS; changes in (d) QF and FOM (e) DL.

Among them, the high-frequency constant ε_{∞} =3.1524 and the plasma frequency $\omega_p = 2\pi \times 0.53 \times 10^{12} \text{ rad/s}$. $\Delta \varepsilon_p = 0.52$, $\gamma = 2 \times \pi \times 25.3 \times 10^9 \text{ rad/s}$ [58], where Teflon [58] can work at $T_0 = 55 \text{ K}$. When $\alpha = 0.05$, q-BIC is excited, and the point with the reflectance peak, as shown in Fig. 5(b). Due to the relationship between asymmetric

parameters in q-BIC and QF [32], this point was selected as the observation point in thickness detection. The movement state of the observation point as the thickness of the sample layer (*d*) varies from 0.5-9.5 μ m is provided in Fig. 5(a). It can be seen from Fig. 5(b) that as *d* increases, the redshift of the spectral line shows a linear relationship.

Frequency points corresponding to the specific thickness are recorded and fitted, and conducted linear regression analysis to obtain the spectral lines in Fig. 5(c), the *S* of RTS is 0.015 THz/µm. The linear expression is $f = -0.015 \cdot d + 1.192$ THz, R² represents the linear fitting degree [57], and R² = 0.996 indicates a good linear relationship [57]. This represents that the THz RTS has good linearity and maintains a linear fitting relationship within 0.5–9.5 µm. From Fig. 5(d), it can be seen that the highest *QF* can reach 478, and the average value can reach 416, indicating a high resolution. This is due to the property of the q-BIC mode which has the finite *QF*. In addition, the highest value of *FOM* is 6.81 and the average value is 5.65. In Fig. 5(e), the *DL* of the RTS remains at a very high value, the minimum value of *DL* is 0.0072, and the average value is 0.0090. These reflect that RTS has superior sensing performance [47]. The RTS has excellent performance and has important application prospects in biological detection and medical treatment.

When $X \neq 0^{\circ}$, q-BIC is excited at $f_2 = 2.455$ THz, which is q-BIC channel 2. When $X = 3^{\circ}$, the highest *QF* of RRIS can reach 13055, as shown in Fig. 4(c) and Fig. 6(c), respectively. The extremely high QF has significant value in the field of sensing, and can be used for air quality detection [47]. When conducting refractive index sensing, the analyte to be measured is considered as an environmental medium, which eliminates the trouble of constructing a gas sensitive layer or setting up a cavity. The refractive index of mixed gases is represented by n, where gas is injected into the RRIS from the flow in port and sprayed out from the flow out port [46]. The working indicators of the RRIS are plotted in Fig. 6(a), as *n* increases from 1.00 to 1.05, the spectral lines continue to redshift. The relationship between gas volume fraction and frequency shift was linearly fitted in Fig. 6(b), S = 0.27 THz/RIU. The peak of q-BIC is plotted in Fig. 6(b) as a spectral line with the red shift of n, showing a linear relationship and extremely sharp peaks, where $f = -0.27 \cdot n + 2.7$ THz and $R^2 = 0.999$. The changes in QF and FOM value at different frequency points are shown in Fig. 6(c). It can be seen that the average QF is 12,614 and the highest value is 13055, indicating a high QF effect. The average FOM value is 1391, indicating that the RRIS has high resolution. The DL of the RRIS is displayed in Fig. 6(d), indicating that the average value of DL is 3.59 \times 10^{-5} and the minimum value is 3.46 \times

 10^{-5} . This indicates that the sensor has a very small *DL* and good performance [57]. It has potential applications in gas quality detection and human health status analysis.

To further demonstrate the ingenuity and excellent sensing performance of the dual channel q-BIC used in sensing design in this paper, Table 1 is plotted.

4. Conclusion

In this paper, a YCSM is proposed. Dual-channel q-BICs are achieved at positions $f_1 = 1.223$ THz and $f_2 = 2.455$ THz, respectively. The q-BIC channels 1 and 2 are respectively affected by the ED and the TD effects. When asymmetry parameters are introduced, BIC degenerates into q-BIC, which has a quite high QF and can be used to design responsive sensors. Sections 1–2 of Supplementary Material provide a detailed manufacturing processing of YCSM. q-BIC channel 1 at f_1 is used to design RTS for fingerprint spectrum analysis. When $\alpha = 0.05$, $R^2 =$ 0.992, S = 0.015 THz/µm, an average QF = 416.1, an average FOM =5.65, average DL = 0.0090. q-BIC channel 2 at f_2 is used to design an RRIS that can monitor the refractive index of gas. When $X = 3^\circ$, $R^2 =$ 0.999, S = 0.27 THz/RIU, an average QF = 12614, an average FOM =1391, $DL = 3.59 \times 10^{-5}$. This design proposes a dual channel q-BIC, which provides a new approach for multitasking devices and is expected to be applied to integrated optical responsive sensing devices.

Ethical approval statement

Following specific guidelines for any research involving humans or animals.

Author contribution

Acknowledgement that all authors accepted the responsibility for the content of the manuscript and consented to its submission, reviewed all the results, and approved the final version of the manuscript.



Fig. 6. (a) Changes in the position of reflection peaks under different n, (b) linear fitting results of the RRIS, (c) QF and FOM values of the RRIS, (d) DL.

Table 1

Comparison of q-BIC channel numbers and sensing performance.

Refs.	q-BIC channel number	Multitasking detection	Physical quantity	QF	FOM	DL
[10]	1	\checkmark	RI	1200	×	$1.00 imes10^{-7}$
[59]	0	×	RI	1105	800	×
[60]	0	\checkmark	Gas	×	×	$8.00 imes10^{-5}$
[61]	1	\checkmark	Biological solution	<10	×	$1.50 imes10^{-2}$
[62]	0	×	Thickness	75.7	64.7	×
This work	2	\checkmark	Thickness	478	6.81	$7.20 imes10^{-3}$
		-	RI	12,614	1391	$3.59\times10^{\text{-5}}$

CRediT authorship contribution statement

Ting-Hao Zhang: Writing – original draft, Resources, Investigation, Formal analysis. Bao-Fei Wan: Visualization, Validation, Software, Resources. Rui-Yang Dong: Software, Resources, Methodology, Data curation. Bing-Xiang Li: Supervision, Funding acquisition. Hai-Feng Zhang: Writing – review & editing, Supervision, Conceptualization.

Informed consent

Informed consent was obtained from all individuals included in this study.

Declaration of competing interest

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

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.matdes.2025.114098.

Data availability

Data will be made available on request.

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