Simulation Study of a Diamond Epithermal Neutron Flux Detector for BNCT

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Abstract

Boron Neutron Capture Therapy (BNCT) is an advanced precision-targeted tumor treatment technology with broad application prospects. One of the core tasks in the development of this technology is the measurement of neutron flux. Current methods for measuring epithermal neutron flux in BNCT neutron beams mainly include the multi-foil activation method and the Bonner sphere spectrometer method, which suffer from cumbersome operational procedures, long measurement times, and inability to perform online real-time measurements, necessitating the development of new detection techniques. This paper employs the Monte Carlo simulation method to design a diamond-based epithermal neutron flux detector for BNCT neutron beam monitoring requirements, equipped with a nuclear electronics readout system to achieve real-time monitoring of epithermal neutron flux. The optimized epithermal neutron detector employs a D2O sphere with a radius of 37 cm and 0.01 cm Fe foil as moderator material and high-energy neutron absorber material, the diamond detector dimensions are 1$×1×$0.03 cm, and 17 m 6Li is selected as the neutron conversion layer. Through performance verification in BNCT radiation fields of accelerator neutron sources and reactor neutron sources, the results demonstrate that the designed detector has a neutron response energy range of 0.5 eV–10 keV, the uncertainty of epithermal neutron flux measurement results is less than 4%, superior to currently used multi-foil activation and Bonner sphere spectrometer methods, enabling high-precision epithermal neutron flux measurement in BNCT radiation fields and providing guidance for subsequent fabrication and testing of the detector.

Full Text

Preamble

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Simulation Study of Diamond-Based Epithermal Neutron Flux Detectors for BNCT

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Abstract

[**Background**] Boron Neutron Capture Therapy (BNCT) is an advanced and precise targeted tumor treatment technology with broad application prospects. One of the core tasks in developing this technology is neutron flux measurement. Current methods for measuring epithermal neutron flux in BNCT beams, primarily the multi-foil activation method and Bonner sphere spectrometry, suffer from complicated procedures, long measurement times, and inability to perform real-time online measurements. Therefore, there is an urgent need to develop new detection technologies.

[**Purpose**] This paper employs Monte Carlo simulation methods to design a diamond-based epithermal neutron flux detector for BNCT beam monitoring, equipped with a nuclear electronics readout system to achieve real-time monitoring of epithermal neutron flux.

[**Methods**] The optimized epithermal neutron detector uses a D_2O sphere with a radius of 37 cm and a 0.01 cm Fe foil as moderator and high-energy neutron absorber materials. The diamond detector dimensions are 1 × 1 × 0.03 cm, with 17 m of ^{6}Li selected as the neutron conversion layer.

[**Results & Conclusions**] Performance verification using BNCT radiation fields from both accelerator and reactor neutron sources demonstrates that the designed detector has a neutron response energy range of 0.5 eV–10 keV, with measurement uncertainty for epithermal neutron flux less than 4%, surpassing current multi-foil activation and Bonner sphere spectrometry methods. The detector can accurately measure epithermal neutron flux in BNCT radiation fields, providing guidance for subsequent detector fabrication and testing.

Keywords: BNCT, Diamond neutron detector, Epithermal neutron sensitivity, Coefficient of variation (CV), Flatness, Monte Carlo simulation

Classification: TL99

Malignant tumors pose a significant threat to public health, and developing diagnostic and therapeutic approaches for malignant tumors represents an important measure to address this critical health challenge. Conventional treatment methods such as surgical resection, radiotherapy, and chemotherapy have achieved certain successes but suffer from incomplete treatment, poor efficacy against metastatic tumors, and severe side effects. Consequently, more selective precision-targeted therapies have become a research focus and technological development direction. High-efficacy targeted radiopharmaceuticals and Boron Neutron Capture Therapy (BNCT) currently represent the most promising precision tumor treatment modalities and are developing rapidly.

BNCT is an emerging and rapidly advancing tumor treatment approach that loads boron-10 onto drug molecules, enabling targeted therapy of cancer cells through their selective uptake of these molecules. The boron-10-containing drug molecules themselves are not radioactive; they undergo nuclear reactions under neutron irradiation to produce high-energy alpha particles with extremely short ranges in human tissue, killing tumor cells while sparing healthy tissue. This safe and efficient precision tumor therapy has attracted widespread attention recently. The reaction cross-section between boron-10 and neutrons follows a 1/v distribution in the low-energy region. To enhance boron drug efficacy, thermal and epithermal neutrons are typically used for irradiation. For deep-seated tumors, thermal neutrons have a mean free path of only a few centimeters in human tissue, making effective treatment difficult. Since epithermal neutron beams (0.5 eV–10 keV) have greater penetration than thermal neutrons (<0.5 eV), they are widely used for deep tumor treatment in BNCT. A key technology in BNCT is neutron flux monitoring for assessing neutron field intensity, treatment planning, and irradiation time determination. Precise measurement of epithermal neutron flux is critical for ensuring therapeutic efficacy and patient radiation safety. Therefore, accurate measurement of epithermal neutron flux in BNCT beams is of great significance.

BNCT neutron sources produce high-flux ($ 10^{9}$ $n \cdot cm^{-2} \cdot s^{-1}$) mixed neutron fields composed primarily of epithermal neutrons but also containing thermal and fast neutron components. These latter components contribute little to therapeutic effect yet severely interfere with epithermal neutron measurement accuracy. Current methods for measuring neutron spectra and flux in BNCT radiation fields mainly include the multi-foil activation method and Bonner sphere spectrometry. For example, Auterinen et al. used the multi-foil activation method to measure neutron field spectra at eight BNCT facilities worldwide, while Masuda et al. employed Bonner sphere spectrometry to measure the neutron spectrum and flux of an accelerator-based BNCT neutron source using the p-^{9}Be reaction, and Chen et al. used Bonner sphere spectrometry to measure the neutron beam spectrum of IHNI-1. However, both methods involve cumbersome procedures, long measurement times, and low precision, failing to meet the development needs of BNCT technology.

Building upon previous research on diamond fast-thermal neutron detectors, this paper designs a novel epithermal neutron detector. Using a diamond neutron detector as the core component with moderator design, the detector achieves real-time monitoring of epithermal neutron flux without requiring neutron spectrum measurement. Diamond consists primarily of carbon, offering high biocompatibility and density similar to human tissue, making its neutron moderation, scattering, and energy deposition processes highly analogous to biological tissue and yielding measurements that better reflect actual biological response. This study employs MCNP5 Monte Carlo simulation to optimize detector structure, neutron response, neutron conversion material selection, moderator material choice, and high-energy neutron resonance absorption strategies. Performance verification using typical BNCT accelerator and reactor neutron source spectra demonstrates that the designed diamond epithermal neutron detector can accurately measure neutron flux in BNCT radiation fields without spectrum measurement.

1 Diamond Material Properties

Diamond is a new-generation high-performance semiconductor material with a bandgap of 5.47 eV, high atomic displacement threshold (~42 eV), strong carbon-carbon covalent bonds, extremely low radiation damage under high neutron/gamma flux, and high electron mobility, making it ideal for high-performance, fast-response, long-life neutron detectors. This study uses diamond as the core detector material, leveraging its ultra-high electron mobility and low defect characteristics to achieve >99% charge collection efficiency and significantly improved neutron detection efficiency. Fast response is realized through high bias voltage and fast electronics, with virtually no response to gamma rays, making the detector insensitive to gamma interference.

1.1 Diamond Detector Working Principle

Diamond neutron detectors indirectly detect neutrons through secondary charged ions produced by neutron nuclear reactions. High-energy secondary charged particles ionize carbon atoms, creating electron-hole pairs that drift toward electrodes under an electric field to form pulse signals. Neutrons can directly undergo the $^{12}C(n,\alpha)^{9}Be$ reaction with diamond, but this reaction has a high threshold energy of 6.17 MeV. For neutrons below 6.17 MeV, neutron conversion materials must be introduced to increase the nuclear reaction cross-section. This study selects ^{6}Li and ^{10}B as neutron conversion materials, utilizing their large thermal neutron absorption cross-sections (^{6}Li: 942 barns, ^{10}B: 3840 barns) to undergo nuclear reactions with thermal neutrons and produce high-energy charged particles such as alpha particles and tritons. These charged particles pass through the conversion layer and ionize the diamond matrix to generate signals.

1.2 Diamond Neutron Detector Structure Simulation

Detector performance is directly determined by parameters such as the neutron conversion layer and diamond layer thickness. Monte Carlo simulation is used to determine thermal neutron detection efficiency. The theoretical calculation model dimensions are 4 × 4 × 0.5 mm, with a 20 nm thick gold layer on the semiconductor surface serving as a contact layer. The conversion layer is placed on top of the gold layer, as shown in Figure 1 [Figure 1: see original paper].

During simulation, energy deposition in the diamond semiconductor material is converted to pulse height. By analyzing the resulting pulse height distribution and setting an appropriate discrimination threshold, neutron detection efficiency is calculated. Only secondary charged particles transported into the semiconductor material contribute to neutron detection. In the simulation, an isotropic thermal neutron point source at 0.0253 eV is placed on the semiconductor surface.

The intrinsic detection efficiency, defined as the ratio of total counts recorded by the detector to the number of neutrons entering it, serves as the primary performance metric. Since low-energy gamma rays and electronic noise typically accumulate in the low-energy region and affect counting, an energy threshold is set (200 keV in this study). While increasing conversion layer thickness facilitates more nuclear reactions and secondary charged particles, the limited range of secondary particles such as α particles (^{4}He), ^{3}H (tritium), and ^{7}Li (lithium) in the conversion material means that continuously increasing thickness enhances self-absorption and reduces particle emission efficiency. Therefore, an optimal conversion layer thickness exists theoretically.

Using a planar detector model and MCNP5 simulation for a point-source thermal neutron incidence scenario, the neutron detection efficiency results are shown in Figure 2 [Figure 2: see original paper]. Both ^{10}B and ^{6}Li conversion layers exhibit optimal thickness values: the optimal ^{10}B thickness is 2 m with 5.57% detection efficiency, while the optimal ^{6}LiF thickness is 17 m with a peak detection efficiency of 5.47%. These results agree well with literature data, with minor differences arising from neutron cross-section database versions or statistical fluctuations. The agreement in trends and limiting efficiencies confirms the validity of the planar detector structure design and simulation. The results show similar detection efficiencies for both materials, but ^{6}Li has a smaller neutron reaction cross-section, requiring greater thickness for maximum efficiency. Its advantage lies in higher reaction energy and longer secondary particle range, allowing more relaxed electrode requirements. In contrast, ^{10}B has a larger thermal neutron cross-section but lower reaction energy, resulting in shorter secondary ion ranges in both conversion material and electrodes, thus requiring thinner electrodes. Additionally, the 480 keV gamma ray released in this reaction introduces extra interference that may further reduce overall detector efficiency in practical applications.

2 Epithermal Neutron Detector Structure Design

This study employs a diamond substrate with conventional dimensions (1×1 cm area, 300 m thickness) and uses a standard moderator material (high-density polyethylene) to ensure flat sensitivity across the epithermal neutron energy range. Monte Carlo simulation is used to obtain optimal parameters including moderator sphere radius, diamond substrate dimensions, and thermal/fast neutron absorber materials and thicknesses.

2.1 Theoretical Model and Methods

Throughout the simulation, the neutron source is set as a monoenergetic parallel plane source incident along the positive X-axis with a 5 cm diameter, ensuring complete detector coverage within the radiation field. To obtain the sensitivity variation with neutron energy in the 0.5 eV–10 keV range, the F4 cell flux tally is used to calculate average neutron flux in target cells, with the calculation model shown in Figure 3 [Figure 3: see original paper].

This work defines the Coefficient of Variation (CV) to quantify the flatness of the detector' s sensitivity curve within the epithermal neutron energy range, facilitating better design of detector dimensions. CV evaluates the degree of variation (dispersion) among observations, defined as the ratio of standard deviation σ to mean value :

For finite sample sizes (10 sampling points collected in the 0.5 eV–10 keV range in this study), sample standard deviation (S) and sample mean ( ) can be used as estimates for σ and , where and S are calculated by:

Thus, for finite sample sizes, the practical application of Equation (1) in this study becomes:

The CV value is related to the dispersion degree of observations; a smaller CV indicates less dispersion and flatter sensitivity curves in the epithermal neutron energy range. Therefore, this study uses CV as a reference for detector design.

2.2.1 Neutron Conversion Material Selection

Based on the simulation results in Section 2.2, the maximum detection efficiencies of ^{10}B and ^{6}Li show no significant difference. To further determine the appropriate conversion layer material and theoretical thickness, the sensitivity of both materials at their optimal thicknesses is compared.

Figure 4 [Figure 4: see original paper] data shows that at optimal conversion layer thickness, the minimum CV values for ^{10}B and ^{6}Li are 11.0% and 10.99%, respectively, with negligible difference. However, considering that ^{10}B's reaction with thermal neutrons introduces gamma interference that complicates subsequent gamma discrimination, and based on market research showing that ^{6}LiF is commercially available at relatively low cost, ^{6}Li is selected as the neutron detector conversion material based on both physical characteristics and market availability.

2.2.2 Neutron Conversion Layer Thickness

After selecting ^{6}Li as the conversion layer material, the effect of conversion layer thickness on sensitivity curve flatness must be determined. Figure 5 [Figure 5: see original paper] shows that varying the conversion layer thickness (13, 15, 17, 19, 21, 23 m) has minimal impact on CVmin, which remains around 11.0%. Excluding simulation errors, conversion layer thickness essentially does not affect sensitivity curve flatness. However, thickness does affect thermal neutron detection efficiency. To ensure optimal detector performance, 17 m of ^{6}Li is selected as the conversion layer thickness for subsequent studies.

2.3.1 Diamond Layer Thickness

Different diamond substrate thicknesses result in different maximum energy deposition capabilities, with thicker sensitive regions yielding higher detection efficiency and affecting epithermal neutron sensitivity curve flatness. Figure 6 [Figure 6: see original paper] shows that varying diamond substrate thickness (100, 200, 300, 400, 500 m) has minimal effect on sensitivity curve flatness. However, increasing thickness improves detection efficiency, while excessive thickness increases cost and gamma ray deposition. Therefore, the commonly used thickness of 300 m is selected for practical requirements.

2.3.2 Diamond Layer Size

This study requires the unidirectional parallel plane source to be much larger than the detector size. Increasing detector size means detecting more neutrons, affecting sensitivity curve flatness. Figure 7 [Figure 7: see original paper] shows that increasing diamond size (1$×1, 1.5×1.5, 2×2, 2.5×2.5*cm*)*slightlyincreasesCVmin.Analysisrevealsthatsm* cm, which is also the commonly available maximum size for commercially purchased diamond wafers.

Having determined conversion layer material and thickness, diamond size, and thickness in Sections 3.2 and 3.3, the data from Figures 5–7 reveal that even with ideal parameters, the flatness sensitivity using polyethylene for neutron moderation remains inadequate, requiring further moderator material optimization.

2.4 Detector Moderator Structure Optimization

In the above studies, 17 m of ^{6}Li was selected as the conversion layer, with diamond substrate dimensions of 1$×$1 cm and thickness of 300 m, using high-density polyethylene as moderator. The ideal CVmin value of 10.8% is far from meeting epithermal neutron sensitivity flatness requirements, necessitating new moderator materials.

2.4.1 Moderator Material Optimization According to neutron reaction cross-section databases, polyethylene’ s neutron absorption cross-section in the low-energy region is two orders of magnitude higher than that of Be or D materials, causing significant absorption of moderated epithermal neutrons. To address this, polyethylene moderators are optimized by replacing high-density polyethylene with Be or D_2O for fast neutron moderation.

Figure 8 [Figure 8: see original paper] shows sensitivity curves using Be and D_2O instead of polyethylene for fast neutron moderation. For Be moderation, the optimal thickness is 26 cm with CVmin = 3.46%. For D_2O moderation, the optimal thickness is 38 cm with CVmin = 4.14% (although 60 cm achieves CVmin = 3.73%, the marginal flatness improvement does not justify the substantial resource consumption). Both materials demonstrate good moderation and sensitivity flattening effects.

2.4.2 Low Sensitivity to Thermal and Fast Neutrons Epithermal neutron detectors must be insensitive to thermal neutrons and higher-energy fast neutrons. This study employs fast neutron and low-energy thermal neutron absorption layers to reduce their sensitivity.

Utilizing the properties of ^{56}Fe and ^{60}Ni, which have large capture cross-sections in the low-energy region and strong resonance absorption in the high-energy region (^{56}Fe resonance absorption cross-section increases by 3 orders of magnitude, ^{60}Ni by 4 orders of magnitude) as shown in Figure 9 [Figure 9: see original paper], appropriate thicknesses of Fe and Ni layers are placed outside the moderator to reduce the fraction of low-energy thermal neutrons and fast neutrons entering the detector. Since epithermal neutron flux constitutes the majority of BNCT neutron beams (Φ_{epi}/Φ_{total} ≥ 0.85), this ensures that detected neutrons are primarily in the epithermal energy range.

Figure 10 [Figure 10: see original paper] shows fast neutron sensitivity calculations for 26 cm Be (optimal moderator thickness) with added absorption layers. The results indicate that Be as a moderator cannot meet the requirement of insensitivity to fast neutrons; adding 0.001–0.05 cm thick Fe and Ni absorption layers fails to reduce fast neutron sensitivity sufficiently. Additionally, beryllium and its compounds are highly toxic and pose environmental hazards to operators and ecosystems. Therefore, D_2O is selected as the moderator material for subsequent studies.

Analysis of optimal flatness curves for different thicknesses of ^{56}Fe and ^{60}Ni (Figure 11 [Figure 11: see original paper]) shows that CVmin values initially decrease then increase slightly with absorption layer thickness. Thin absorption layers capture low-energy thermal neutrons and resonantly absorb fast neutrons, concentrating collected neutrons in the epithermal region and yielding more uniform sensitivity distribution. Overly thick absorption layers cause excessive capture and resonance absorption, creating a sensitivity distribution that is high in the middle and low on both sides, while multiple scattering of fast neutrons in thick layers may generate "secondary epithermal neutrons" causing spectral mixing and reduced flatness. Figure 11 data analysis shows that Fe as an absorber material yields lower CVmin values and higher epithermal neutron sensitivity curve flatness. Fe is therefore selected as the absorption layer material.

Figure 12 Figure 12: see original paper describes three absorption layer and moderator parameter configurations (optimal moderator thicknesses of 39 cm, 37 cm, and 37 cm for 0.001 cm, 0.005 cm, and 0.01 cm Fe foil thicknesses, respectively). These configurations suppress thermal and fast neutron sensitivity to low levels while maintaining flatness. The 39 cm D_2O configuration shows lower average sensitivity than the 37 cm configuration due to excessive self-absorption. The 0.01 cm and 0.005 cm absorption layers show similar suppression capabilities for thermal and fast neutrons, but the 0.01 cm Fe layer yields a lower CVmin value. With 37 cm D_2O + 0.01 cm Fe, CVmin = 2.56%, making this the optimal configuration. The final optimal structure uses a 37 cm radius D_2O sphere + 0.01 cm Fe foil for effective thermal and fast neutron absorption, diamond substrate of 1 × 1 × 0.03 cm, and 17 m of ^{6}Li as the neutron conversion layer material, as shown in Figure 13 [Figure 13: see original paper].

Figure 12(b) demonstrates that the designed detector is sensitive to epithermal neutrons with a flat sensitivity curve in this energy range while maintaining low sensitivity to thermal and fast neutrons, indicating its capability to accurately measure epithermal neutron flux in BNCT neutron beams.

2.5 Performance Testing Based on Simulated BNCT Radiation Fields

To further verify the performance of the designed BNCT epithermal neutron detector, simulated BNCT radiation fields are constructed based on domestic and international research findings, and detector performance is tested using Monte Carlo simulation methods.

Commonly used neutron sources in BNCT research and clinical applications include nuclear reactors and accelerator devices. All clinical trials to date have been conducted using reactor neutron sources, as reactors can provide the high-flux neutron beams required for therapy. However, reactors have significant limitations for clinical use, including lack of supporting medical facilities, high construction and operational costs, and difficulty ensuring patient safety during treatment. In recent years, accelerator-based neutron sources have attracted increasing attention for their suitability in hospital environments and have become an important direction for BNCT clinical translation. Many countries and regions (including Japan, Finland, the UK, Russia, Italy, Argentina, and Taiwan, China) are actively developing accelerator-based neutron source devices and supporting systems. Accelerator neutron sources offer advantages including flexible control, concentrated energy distribution, minimal accompanying gamma contamination, lower construction costs, and higher safety, enabling widespread deployment in urban hospitals. However, their relatively lower neutron flux and less directional/collimated beams compared to reactor sources require further investigation.

Since both neutron source types are widely used in current research, this study validates the designed epithermal neutron flux detector using reactor-based BNCT neutron beams and accelerator-based BNCT neutron beams (based on D-D, D-T, and p-^{7}Li reactions). The BNCT beam energy spectra used in the simulation calculations are shown in Figure 14 [Figure 14: see original paper]. For each BNCT therapeutic beam, the measured epithermal neutron flux Φ' _{epi} is calculated by:

Φ' _{epi} = R/

where R = Y × Φ_{total} is the reaction rate induced by each BNCT therapeutic beam (units: cps; Y is calculated by Monte Carlo in units of $cps/(n/cm^2/s)$; Φ_{total} is the total neutron flux), and = 3.9008×10^{-7} $cps/(n/cm^2/s)$ is the normalized average sensitivity of the detector in the epithermal neutron energy range.

The uncertainty of Φ' _{epi} is:

δ{epi} = |Φ' {epi} - Φ_{epi}| / Φ_{epi}

where Φ_{epi} is the actual epithermal neutron flux of each boron neutron capture therapy beam.

The diamond epithermal neutron detector is used to validate the aforementioned neutron sources. Based on the described calculation methods and conditions, Φ' *{epi} and δ*{epi} are calculated for four radiation fields, with results shown in Table 1 . For comparison, the actual epithermal neutron flux Φ_{epi} of the corresponding BNCT neutron fields is also included in Table 1. The data show that the measurement uncertainty for epithermal neutron flux is less than 4%, superior to current multi-foil activation and Bonner sphere spectrometry methods, demonstrating that the designed detector can accurately measure epithermal neutron flux in BNCT neutron beams.

The primary cause of measurement deviation is the contribution of neutron counts from the fast and thermal neutron energy regions. Neutrons in the 10^4-10^6 eV range and 0.01-0.5 eV range still exhibit certain sensitivity, leading to measurable responses in these energy regions and resulting in deviation. The Fe foil provides good fast neutron absorption capability, controlling the sensitivity to 1 MeV fast neutrons at 2.37×10^{-7} $cps/(n/cm^2/s)$, a significant reduction compared to the epithermal neutron sensitivity = 3.9008×10^{-7} $cps/(n/cm^2/s)$ (the normalized average sensitivity in the epithermal neutron energy range). Further improvements in fast neutron absorption capability through modified absorber materials may achieve sensitivity exclusively to epithermal neutrons.

3 Conclusion

This study employs Monte Carlo simulation to optimize diamond neutron detector structural parameters. Using ^6Li and ^{10}B as neutron conversion materials, optimal detection efficiencies for a 0.0253 eV thermal neutron point source are 5.47% and 5.57%, respectively, validating the feasibility and effectiveness of the simulation structure design. For epithermal neutron flux measurement, a high-density polyethylene spherical moderator is placed outside the diamond neutron detector, with 17 m of ^6Li selected as the conversion layer and diamond substrate dimensions of 1 × 1 cm and thickness of 300 m. To further reduce CV values, Be and D_2O are used instead of polyethylene to achieve high-level sensitivity flattening. To meet the design requirement of sensitivity only to epithermal neutrons while being insensitive to thermal and fast neutrons, a

0.01 cm Fe foil is added outside the moderator to eliminate fast and low-energy thermal neutron effects through resonance absorption and capture reactions. The final optimal moderator and absorber configuration is a 37 cm radius D_2O sphere + 0.01 cm Fe foil. Validation tests against simulated accelerator and reactor neutron source radiation fields show uncertainties of approximately 3% in the 0.5 eV–10 keV range, surpassing current multi-foil activation and Bonner sphere spectrometry methods.

The BNCT epithermal neutron flux detector designed in this study is well-suited for real-time measurement of BNCT radiation field characteristic parameters and shows promising application prospects for accurate evaluation of BNCT neutron source quality and precise treatment planning.

Author Contributions: Zhang Ying completed the main research work, including simulation design, MCNP simulation, and manuscript writing; Yan Qiang proposed the research concept; Wu Zhengxin provided theoretical guidance; Lin Shuxian and Gan Yujing assisted with manuscript compilation; Liu Guoqing coordinated project planning and was responsible for manuscript revision.

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Note: Figure translations are in progress. See original paper for figures.