

Multidimensional physical unclonable function encryption architecture based on microtexture in polycrystalline diamond

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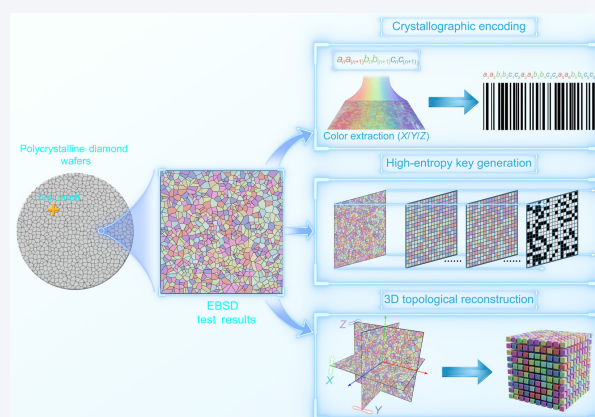
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 Cite this article: Nano Research, 2026, 19, 94908855. <https://doi.org/10.26599/NR.2026.94908855>

ABSTRACT: Conventional physical unclonable functions (PUFs), although delivering unique and non-replicable identifiers for hardware security authentication and key component anti-counterfeiting applications, struggle to provide long-term reliable support under extreme environments such as nuclear reactors, fusion devices, and space radiation, which feature intense radiation and high temperatures. Here, we report a highly robust PUF architecture derived from the intrinsic crystallographic disorder of polycrystalline diamond microtextures. By analyzing electron backscatter diffraction (EBSD) patterns, a multidimensional security framework is established that integrates three complementary encoding dimensions: multi-base numerical conversion of individual microtexture features for primary key generation; three-dimensional topological reconstruction through fusion of single- and multi-directional EBSD maps; and crystallographic coding based on the statistical distribution of (100), (110), and (111) lattice planes. Together, these elements form a three complementary encoding dimensions with exceptionally high entropy and unclonability. To enable deployment across heterogeneous application scenarios, both rigid polycrystalline diamond substrates and self-supported flexible diamond films are developed. The rigid architecture provides ultrahard chemically inert planar security for chip-level authentication, while the flexible diamond films combine curvature adaptability with extreme durability, enabling secure labeling of complex and deformable surfaces such as medical devices. Sharing a unified microtexture-based encoding mechanism, their complementary platforms establish a versatile security solution that seamlessly integrates rigidity and flexibility for high-value electronic components and advanced anti-counterfeiting applications.

KEYWORDS: physical unclonable function (PUF), polycrystalline diamond, microtexture-based encryption, electron backscattering diffraction (EBSD), crystallographic encoding



1 Introduction

In an increasingly interconnected global economy, the proliferation of counterfeit electronic components and substandard pharmaceuticals has become a critical challenge, resulting in substantial economic losses and posing serious threats to public health and societal trust [1–5]. Most conventional anti-

counterfeiting measures, such as barcodes, quick response (QR) codes, and cryptographic identifiers, predominantly rely on external verifiable information carriers to establish authenticity. Despite their widespread adoption, these methods are intrinsically vulnerable: the encoded information is static and can be duplicated or reverse-engineered. Once a label is forged or a digital key is compromised, the entire authentication framework collapses, as security is rooted in data secrecy rather than in the uniqueness of the physical carrier itself [6–8].

Physical unclonable functions (PUFs) have therefore emerged as a fundamentally different paradigm for secure authentication. By leveraging uncontrollable and irreproducible microscopic variations during material fabrication, PUFs generate unique physical “fingerprints” that are extremely difficult—if not theoretically

Received: April 8, 2026; Revised: May 18, 2026

Accepted: May 19, 2026

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impossible—to replicate. Unlike traditional identifiers, PUFs embed security directly into the inherent randomness of the physical world, decoupling authentication from stored information and dramatically increasing the cost and complexity of counterfeiting [9–13]. This intrinsic, hardware-level security has positioned PUFs as a cornerstone technology for next-generation information protection, anti-counterfeiting, and trusted identification systems. However, the effectiveness of a PUF ultimately depends on the nature and stability of its physical entropy source.

Despite significant advancements in PUF technology, existing approaches still suffer from fundamental limitations: Their reliance on a stimulus-response mechanism makes the entropy source highly susceptible to environmental disturbances, aging effects, and security attacks. Specifically, optical PUFs are prone to interference from environmental factors such as temperature and humidity [14, 15], while electrical PUFs face issues including voltage fluctuations and device aging degradation [16–18]. These stability shortcomings severely restrict the long-term reliable application of PUFs in harsh environments.

Against this backdrop, microtexture-based PUFs have gained increasing attention as an alternative strategy. Rather than introducing artificial randomness, these systems directly harness intrinsic microscopic features of object surfaces (such as grain structures, fiber networks, or crystalline textures) as natural entropy sources. This approach eliminates the need for additional fabrication steps or coatings, offering cost-effective, scalable production and non-contact authentication via machine vision [19–22]. Nevertheless, the choice of carrier material remains a critical bottleneck. Conventional substrates, including metals, paper, and organic polymers suffer from oxidation and corrosion, moisture-induced deformation, photo- and thermal degradation, and mechanical wear, leading to irreversible degradation of surface microtextures, and consequently, loss of authentication fidelity over time [23–26]. Therefore, there is an urgent need to develop a novel entropy source carrier with intrinsic stability to fundamentally overcome the above limitations.

Diamond, with its unparalleled physical and chemical robustness, represents an ideal platform to overcome these limitations. As the hardest known natural material, diamond exhibits exceptional resistance to mechanical abrasion and wear. Its dense sp^3 carbon lattice provides extraordinary chemical inertness, enabling resistance to strong acids, bases, and high-temperature oxidation, while its ultrahigh thermal conductivity and radiation tolerance suppress microstructural distortion under extreme environments [27–29]. These attributes uniquely position diamond as a carrier for microtexture-based PUFs capable of maintaining stable, high-fidelity fingerprints over extended timescales, even under harsh operational conditions.

Here, we report a diamond-based PUF architecture constructed from the electron backscatter diffraction (EBSD) patterns of polycrystalline diamond, establishing a multi-dimensional encryption framework that transforms crystallographic disorder into a robust entropy source. By extracting inverse pole figure (IPF) maps along the X , Y , and Z crystallographic directions, as well as their superimposed states, we systematically quantify spatial variations in lattice orientation. These data enables a three complementary encoding dimensions: (i) crystallographic encoding based on the statistical distribution of key lattice planes ((100), (110), and (111)); (ii) high-entropy digital key generation via multi-base numerical conversions of IPF information; (iii) three-

dimensional (3D) topological reconstruction that yields a stereoscopic PUF structure with intrinsic spatial complexity. Notably, we further demonstrate flexible polycrystalline diamond substrates and successfully replicate the entire encryption process, extending the applicability of ultrahard PUF carriers to wearable devices, curved surfaces, and deformable security labels.

By converting microscopic crystallographic randomness into a hierarchical, multidimensional security architecture, this work introduces a disruptive pathway for integrating physical and information security. The resulting diamond-based PUFs offer exceptional environmental resilience, long-term stability, and unclonability, providing a compelling foundation for high-security authentication in advanced security systems, future quantum information carriers and cross-scale anti-counterfeiting technologies.

2 Results and discussion

Leveraging diamond's exceptionally physicochemical stability that ensures long-term preservation of surface microtexture, and harnessing the intrinsically disordered crystalline phases that form spontaneously during polycrystalline diamond growth, this study establishes diamond as an ideal platform for constructing robust PUFs. As illustrated in Fig. 1 and Fig. S1 in the Electronic Supplementary Material (ESM), EBSD characterization of polycrystalline diamond yields IPF datasets that enable the development of three distinct and complementary cryptographic pathways. First, crystallographic encoding is achieved by extracting the spatial distribution features of specific lattice planes from IPFs to generate unique cryptographic signatures (upper). Second, multi-digit conversion transforms IPF data into numerical sequences across multiple bases, enabling the construction of high-entropy one-dimensional PUF keys (middle). Third, 3D PUF architectures are realized via either volumetric reconstruction from individual IPFs or cross-dimensional fusion of multiple IPFs, producing stereoscopic anti-counterfeiting structures with pronounced spatial complexity (bottom). Collectively, this microtexture-based “single-material-multicode” encryption strategy enables the simultaneous derivation of crystallographic codes, multi-digit keys, and 3D PUFs—a triple-layer security mechanism—from a single microstructural dataset. By systematically transforming intrinsic crystallographic disorder into multidimensional, multilevel, and multiform cryptographic carriers, this approach establishes a new paradigm for physical unclonability, substantially enhancing robustness against cloning attacks and cryptographic key space complexity.

To accommodate diverse application scenarios, both rigid (Fig. 2(a)) and flexible (Fig. 2(f)) polycrystalline diamond films were successfully fabricated. X-ray diffraction (XRD, Figs. 2(b) and 2(g)) and Raman spectroscopy (Figs. 2(c) and 2(h)) confirm the formation of the diamond phase in both samples. Except for silicon substrate reflections observed in the flexible film, the diffraction patterns exhibit only characteristic diamond peaks, while Raman spectra show the signature diamond mode at approximately 1332 cm^{-1} . Notably, the flexible diamond film shows a substantially broader Raman peak, with a full width at half maximum (FWHM) of 6.59 cm^{-1} , compared with 2.54 cm^{-1} for the rigid film (insets in Figs. 2(c) and 2(h)). This broadening indicates slightly reduced crystallinity due to rapid growth kinetics and constrained crystal integrity required to achieve controlled thickness and mechanical flexibility [30–32].

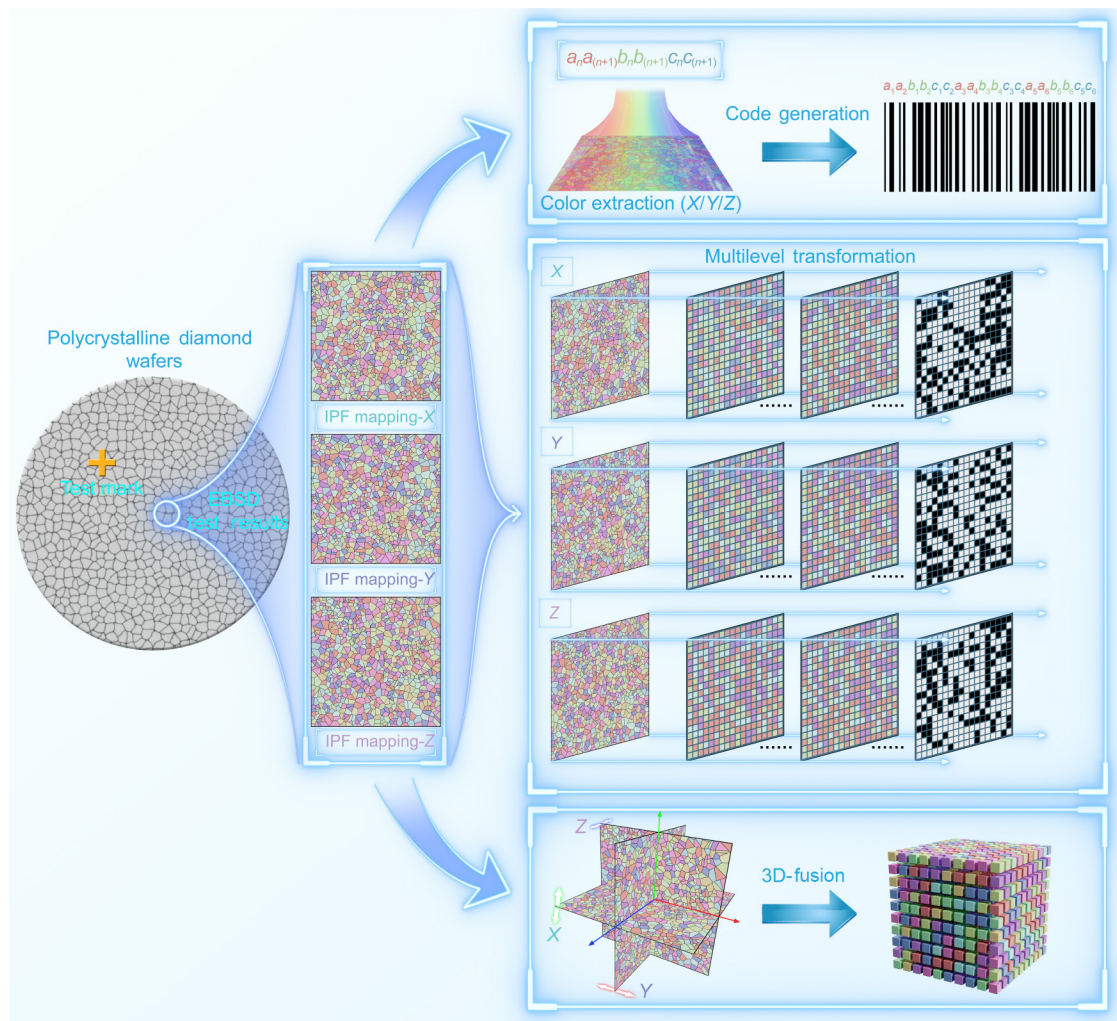


Figure 1 Conceptual framework of multidimensional PUFs based on polycrystalline diamond microtexture. Top: crystallographic encoding derived from statistically distributed lattice orientations. Middle: multi-base numerical conversion encoding of IPF data. Bottom: 3D topological reconstruction encoding enabled by multi-directional crystallographic information.

Surface roughness, as a critical parameter for reliable EBSD analysis, was carefully evaluated. As shown in Figs. 2(d) and 2(i), the polished rigid polycrystalline diamond (RMS = 0.49 nm) and the as-grown flexible diamond film (RMS = 1.81 nm) both exhibit surface roughness values far below the threshold typically required for high-quality EBSD measurements (RMS < 50 nm) [33–35]. Such ultra-smooth surfaces effectively suppress signal distortion and indexing failure, thereby ensuring accurate crystallographic orientation mapping. EBSD orientation maps (Figs. 2(e) and 2(j)) were subsequently obtained, generating IPFs to the sample coordinate axes (X, Y, and Z) as well as a merged orientation map (Figs. S2 and S3 in the ESM), denoted as IPF-X, IPF-Y, IPF-Z, and IPF-C, respectively. The IPF color-coding reflects crystallographic orientations such as [001], [101], [111], and directly reveals pronounced grain size differences between the two samples. In particular, the flexible film exhibits significantly finer grains, which can be attributed to the high nucleation density and constrained grain growth required for rapid film formation in ultrathin flexible structures, as observed by Chu et. al previously [36]. The finer grain structure observed in the flexible diamond films increases both grain-boundary density and crystallographic orientation transition frequency within a given scanning area, thereby increasing the

spatial complexity and entropy density of the resulting PUF patterns. At the same time, because the entropy source originates from lattice-embedded crystallographic organization within diamond, the reduced grain size does not compromise long-term structural stability. The exceptional mechanical hardness and chemical inertness of diamond ensure robust preservation of the microtexture-derived entropy architecture.

To further enhance the encryption complexity of the PUFs, we introduce M -ary encoding strategy ($M \in \{2, 4, 8, 16, 32\}$) leveraging the intrinsic stochasticity of polycrystalline diamond microtextures derived from EBSD IPFs for multi-bit conversion. The quantization workflow initiates with adaptive bottom-label cropping, in which row-gradient detection and red-green-blue (RGB) masking iteratively eliminate annotation regions while ensuring residual text coverage remains below 0.1%. In the present work, the IPF maps encode crystallographic orientations using RGB-based color mapping. However, direct utilization of individual RGB channels may introduce unwanted variations associated with hue and saturation, which are not directly related to genuine orientation contrast. To address this, the processed RGB images were converted into the CIE Lab color space, where the luminance channel (L) was selected as the quantization reference. This channel more effectively

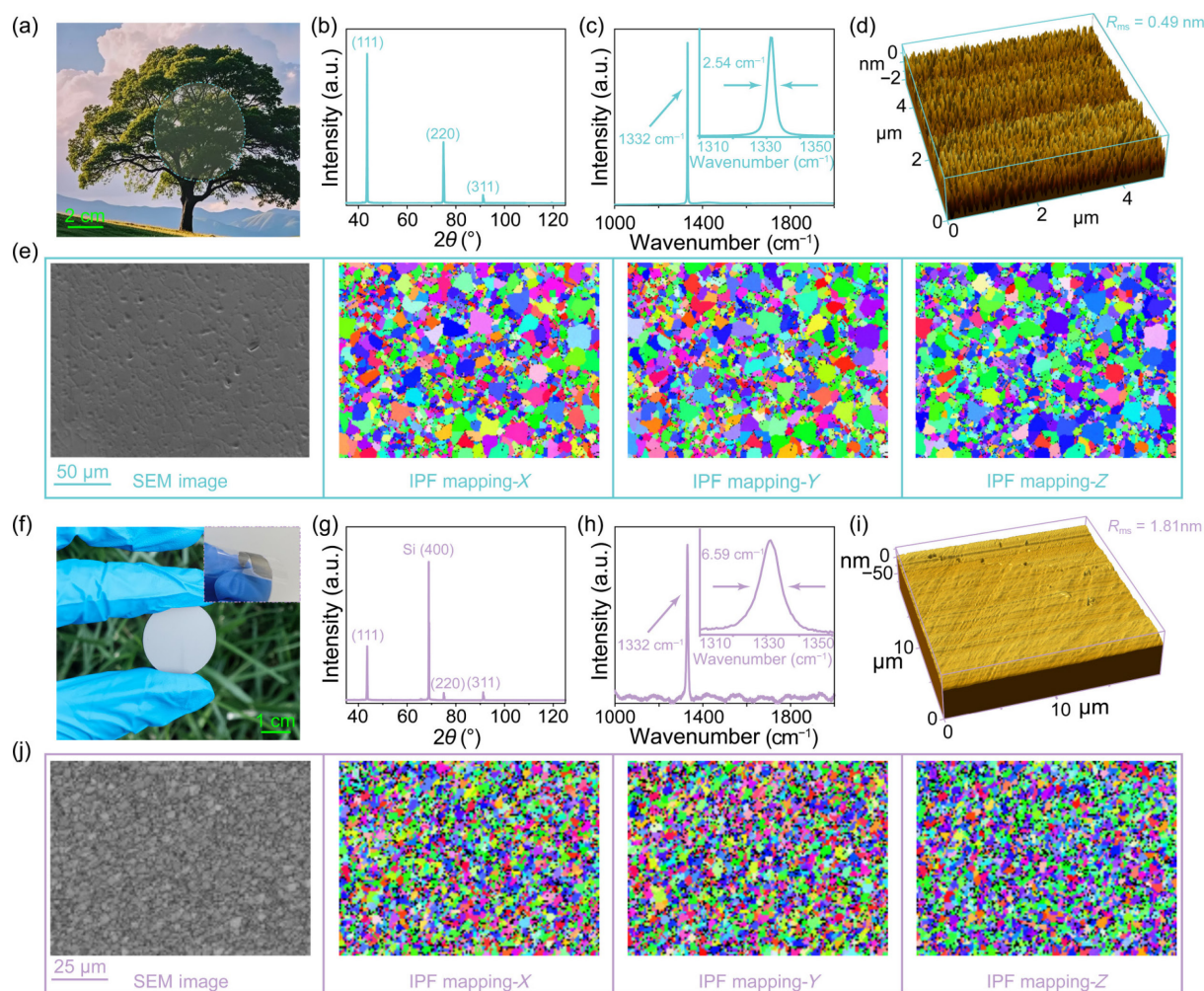


Figure 2 Structural and morphological characterization of rigid and flexible polycrystalline diamond. Rigid 2-inch polycrystalline diamond wafer: (a) optical photograph, (b) XRD pattern, (c) Raman spectrum, (d) AFM height image, and (e) SEM image with corresponding EBSD orientation maps (scale bar, 50 μm). Flexible polycrystalline diamond film: (f) optical photograph, (g) XRD pattern, (h) Raman spectrum, (i) AFM height image, and (j) SEM image with corresponding EBSD orientation maps (scale bar, 50 μm).

captures the overall intensity contrast of the crystallographic microtexture and significantly reduces the influence of minor color fluctuations during EBSD acquisition, thereby improving the stability and consistency of the quantization process for multidimensional PUF encoding. Equal-frequency quantization partitions the sorted L values into K discrete levels ($K \equiv M$), generating an integer label matrix with statistically equivalent pixel counts per level. Final outputs include: discrete pseudocolor maps (via listed colormap), CSV-formatted label matrices (compatible with Origin-based statistical analysis), and quantization fidelity reports validated through mutual information metrics. By prioritizing uniform data distribution, this workflow enhances 3D reconstruction robustness and cross-sample statistical comparability, establishing a technical foundation for microstructure-driven PUF key generation.

Figures 3(a)–3(e) show representative M -ary encoded matrices derived from IPF-X maps. The left and middle columns correspond to two independent measurements of the same PUF, while the right column corresponds to one measurement from a different PUF. All matrices exhibit highly chaotic and intricate distributions, characteristic of strong physical randomness. To validate the feasibility of M -ary encoding, Hamming distance (HD) analysis was

performed (Figs. 3(f)–3(j)). The inter-class HD histograms for binary, quaternary, octal, hexadecimal, and duotrigesimal encodings all conform to Gaussian distributions with mean values of 0.475, 0.738, 0.862, 0.925, and 0.963, respectively. These values closely approximate their theoretical ideals (0.5, 0.75, 0.875, 0.9375, and 0.96875), confirming exceptional uniqueness of the labels under multi-base encoding schemes. Consistent behavior is observed for IPF-Y, IPF-Z, and IPF-C maps (Figs. S4–S6 in the ESM), underscoring the generality of the encoding strategy.

Notably, the information entropy of the resulting PUF codes increases monotonically with the code element length (Figs. S7 and S8 in the ESM), providing a pathway to achieve high coding capacity. This trend corroborates the strong chaos and inherent unpredictability of PUF encoding. However, repeatability analysis reveals that intra-class HD values deviate from the ideal value of zero and increase with code element length (Figs. 3(k)–3(n)), potentially leading to elevated bit error rates (BER) during authentication. Such deviations arise from inevitable perturbations during acquisition, including instrumental drift, subtle sample state variations, and data processing noise. Because longer code elements reduce tolerance to minor assignment errors, HD—defined as the numbers of mismatched symbols in equal-length strings—becomes

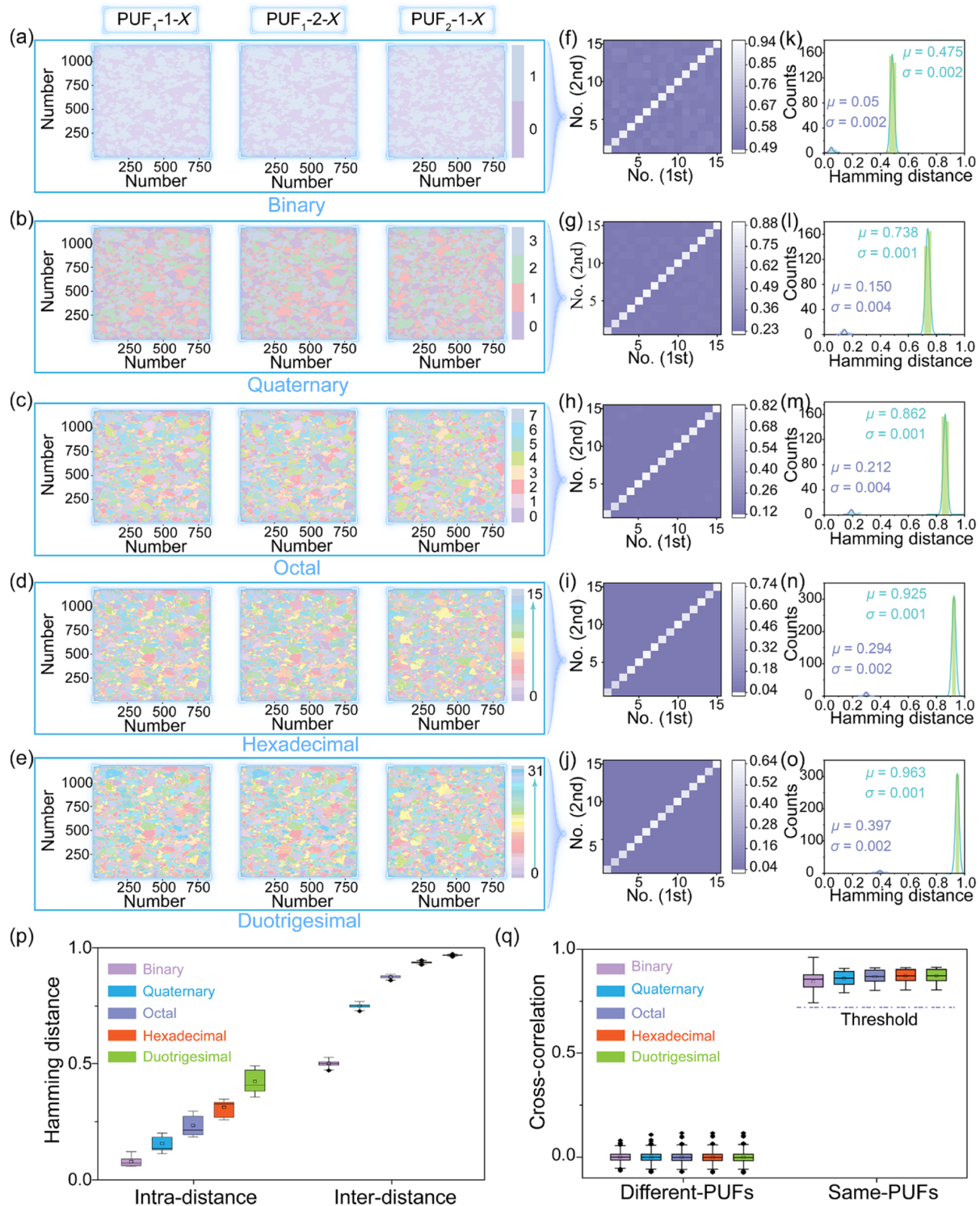


Figure 3 Multi-base conversion PUF derived from polycrystalline diamond microtexture. M -ary encoding matrices generated from IPF- X maps of two measurements of PUF₁ (left and middle) and one measurement of PUF₂ (right), using (a) binary, (b) quaternary, (c) octal, (d) hexadecimal, and (e) duotrigesimal encoding schemes (resolution: 1185 pixel $\times$ 835 pixel). Data labels follow the format “PUF _{i} - j - k ”, where i denotes the PUF instance index, j the measurement repetition, and k the crystallographic parameter ($k = X, Y, Z$, or C). (f)–(j) Pairwise cross-correlation functions for 15 distinct PUFs across first and second measurements under different M -ary encoding. (k)–(o) Statistical distribution of inter- and intra-HDs for 15 distinct PUFs under each encoding scheme. (p) and (q) Box plots summarizing HDs and cross-correlation values as a function of encoding base.

increasingly unsuitable for evaluating repeatability in M -ary PUF systems. To overcome this limitation, we introduce the cross-correlation function (range: -1 to 1) as an alternative metric, which directly quantifies the linear correlation between encoded

sequences: values approaching ± 1 indicate strong correlation, while values near zero denote randomness. Comparative statistical analysis using box plots (15 distinct PUF tags per test group) demonstrates that the cross-correlation function provides

substantially improved repeatability discrimination relative to HD, as shown in Figs. 3(p) and 3(q). In practical applications, where minor raw data deviations from equipment interference or environmental factors are unavoidable, the substantial divergence in cross-correlation coefficients allows scenario-specific adjustment of verification thresholds to ensure high validation success rates. Collectively, the developed *M*-ary PUF encryption framework delivers an adaptable and robust anti-counterfeiting solution for real-world anti-counterfeiting applications.

Building on the insights gained from single-axis multi-base encoding, we next extend the framework from axis-specific optimization to multi-axis synergistic enhancement through quaternary conversion applied to the full 3D microtexture of polycrystalline diamond. As illustrated in Figs. 4(a)–4(d), quaternary encoding is performed on four-dimensional maps (IPF-X, IPF-Y, IPF-Z, IPF-C), where the left and middle columns demonstrate reproducibility validation from two tests of PUF₁, and the right column shows an independent measurement of PUF₂, jointly confirming the process consistency of crystallographic orientation encoding. Cross-orientation statistical validation further substantiates the core security attributes of diamond microtexture-based PUFs. In intra-orientation autocorrelation analysis (Figs. 4(e)–4(j)), repeated measurements along the same orientation axis yield average similarities exceeding 85% (intra-HD ≈ 0.15), confirming exceptional stability in homogeneous PUF measurements. In contrast, homogeneous-orientation comparisons across different PUFs show sharply reduced similarity of $\sim 25\%$ (inter-HD ≈ 0.75). Notably, the cross-orientation correlation analysis (Figs. 4(k), 4(m), and 4(o)) reveals a striking decoupling behavior: similarity between hetero-oriented pairs (e.g., IPF-X vs. IPF-Y) remains statistically indistinguishable whether the measurements originate from the same or different PUFs. This

phenomenon is quantitatively validated in statistical distributions (Figs. 4(l), 4(n), and 4(p)), where cross-orientation HD values remain stabilized at ~ 0.74 , independent of PUF homogeneity/heterogeneity. These properties culminate in the comprehensive boxplot (Fig. 4(q)), demonstrating how orientation-driven entropy decoupling enables a single PUF test region to generate three orthogonal cryptographic keys, exponentially expanding the CRP space and erecting a physically unclonable barrier against correlation attacks. Analogous results obtained using binary, octal, hexadecimal, and duotrigesimal encoding are presented in Figs. S9–S20 in the ESM, demonstrating similar behavior across encoding bases. Additional consecutive testing on the same region (Figs. S21–S25 in the ESM) further confirms the stability of the multidimensional encoding scheme.

Notably, PUF technology is evolving from traditional two-dimensional (2D) architectures toward 3D architectures. By incorporating entropy integration in the vertical dimension, 3D PUFs can enhance entropy capacity and resistance to attacks, thereby achieving a substantial improvement in security [37–39]. To address the complexity and cost challenges associated with 3D manufacturing processes, algorithmic virtualization approaches offer a practical and feasible pathway by simulating 3D interaction characteristics on 2D hardware. Building on this development trend, we propose a reconstruction algorithm that effectively extends 2D texture features into three-dimensional space. In the reconstruction process, two primary assumptions are adopted: (i) 2D crystallographic microtextures can be spatially extended along the third dimension while preserving orientation-derived entropy characteristics; and (ii) orthogonal IPF projections contain complementary orientation-space information that can be integrated into a unified volumetric entropy architecture. Through multi-stage spatial mapping, this approach achieves a dimensional

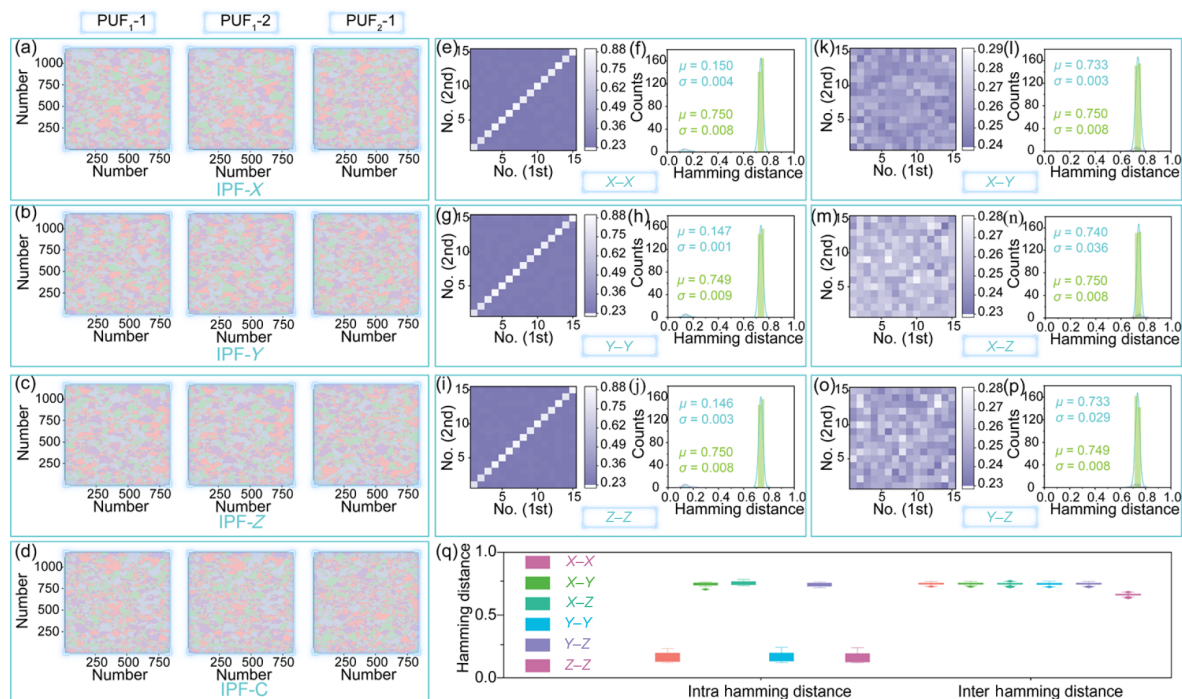


Figure 4 Multidimensional quaternary-encoded PUF based on crystallographic orientation space. (a)–(d) Quaternary encoding results derived from IPF-X, IPF-Y, IPF-Z, and combined IPF-C maps, obtained from two measurements of PUF₁ (left and middle) and one measurement of PUF₂ (right). (e), (g), (i), (k), (m), and (o) Pairwise cross-correlation analyses among 15 distinct PUFs for identical and cross-dimensional comparisons (X-X, Y-Y, Z-Z, X-Y, Y-Z, and Z-X). (f), (h), (j), (l), (n), and (p) Corresponding statistical distributions of inter- and intra-HDs. (q) Box plot summarizing HDs with quaternary encoding across different comparison dimensions.

leap, thereby overcoming the physical limitations of planar structures under existing process conditions and opening an important breakthrough direction for next-generation high-reliability anti-counterfeiting systems that leverage the exceptional stability of diamond materials. In this study, 3D reconstruction pipeline generates structured voxel models through algorithmic spatial expansion of 2D images: Initially, raw or quantized colormap inputs undergo adaptive resolution preprocessing-based on the image's shorter edge dimension, a unified size N (multiple of 32 within [192, 384]) is algorithmically selected, with aspect ratio preserved via padding/cropping to balance computational efficiency and detail retention. Subsequently, single-plane extrusion replicates the 2D image along a specified axis ($X/Y/Z$) into an $N \times N \times N$ voxel volume, modulating intensity via depth distribution profiles (uniform filling, Gaussian attenuation, or linear fade-out). Triplanar fusion then eliminates axial distortion by orthogonally projecting three directional maps and blending color values through spatial position-weighted mixing. Finally, occupancy threshold filtering dynamically eliminates low-intensity noise voxels, enabling four visualization outputs (scatter plots for macrostructure, complete voxel cubes, boundary extraction, multi-face textured cubes), achieving intelligent dimensional reconstruction from 2D pixels to 3D structures.

Figure 5 and Fig. S26 in the ESM present the results of 3D topological reconstruction based on polycrystalline diamond microtexture, focusing on processing and fusing IPF from individual directions (IPF-X, IPF-Y, IPF-Z, IPF-C) to construct 3D PUFs with high stability and uniqueness. Figures 5(a), 5(d), and 5(g), and Figs. S27–S30 in the ESM detail the single-direction

reconstruction process: starting from IPF color texture maps of the X , Y , Z , and C directions, steps include binarization (converting continuous textures to binary feature maps), uniformization (standardizing feature sizes to eliminate scale differences), and finally 3D reconstruction to generate respective 3D PUFs (small cubes on the right, representing each direction's topological structure). Figures 5(b), 5(e), and 5(h) show cross-correlation function comparisons of two measurements for 15 different PUFs (same direction, e.g., IPF-X vs. IPF-X), with highly overlapping curves (correlation coefficients > 0.85) indicating high repeatability for the same PUF. Figures 5(c), 5(f), and 5(i) present the statistical distributions of intra-HD derived from 15 distinct PUFs (intra-HD, between two measurements of the same PUF, reflecting stability—smaller values are better) and inter-HD (between different PUFs, reflecting uniqueness—values closer to 0.5 are better). Results show intra-HD concentrated in low-value regions (e.g., < 0.1) and inter-HD distributed around 0.488, validating the unclonability of single-direction PUFs. Figure 5(j) is a boxplot of HD for 3D stereoscopic PUFs reconstructed from binary/quaternary single-direction IPFs, quantifying the stability and uniqueness of single-direction 3D PUFs. Figures S31–S35 in the ESM demonstrate the process and results of constructing quaternary 3D PUFs through 3D reconstruction of microtexture images from the X , Y , Z , and C directions of the same PUF, which also exhibit this pattern.

Figure 5(k) and Fig. S36 in the ESM illustrate the fusion reconstruction process for $X/Y/Z$ IPFs: integrating texture information from all three directions, followed by the same binarization/uniformization steps, yields more complex 3D PUFs (large cube on the right, showing multi-directional fusion

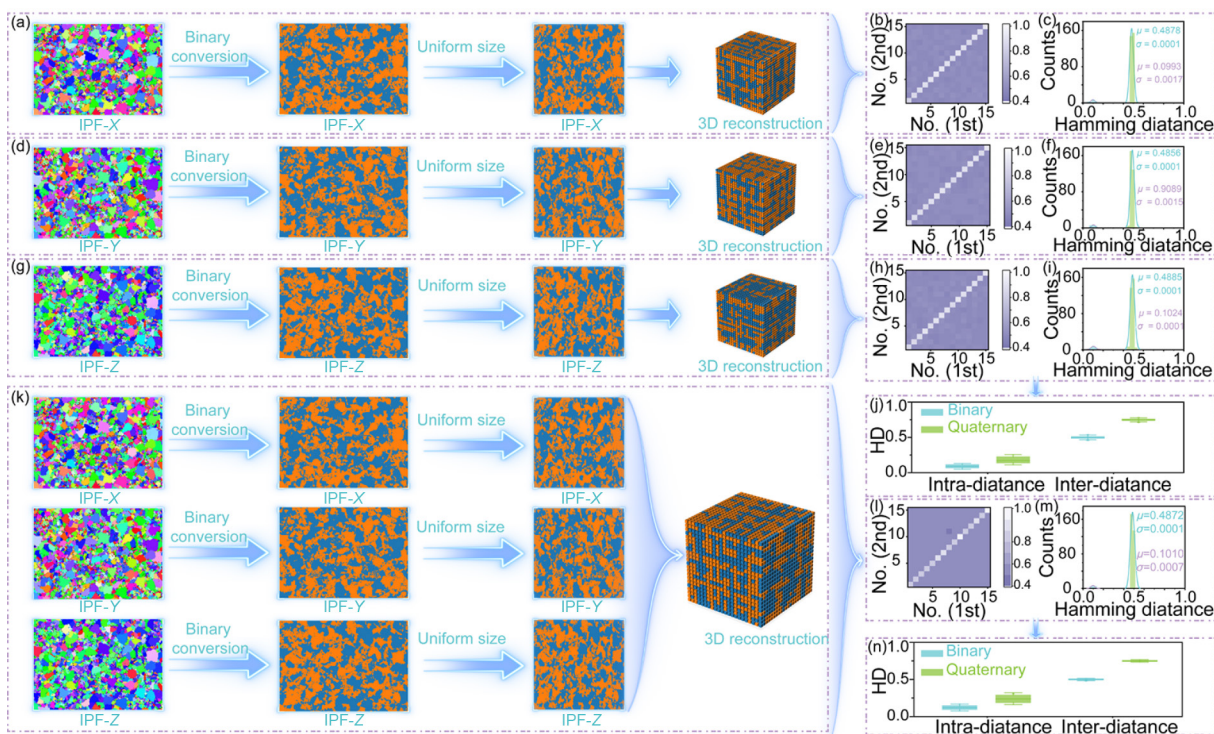


Figure 5 Three-dimensional topological reconstruction of stereoscopic PUFs. (a), (d), and (g) Construction and visualization of binary 3D PUFs through spatial reconstruction of microtexture images from the X , Y , and Z crystallographic directions of the same PUF. (b), (e), and (h) Pairwise cross-correlation analyses for 15 PUFs across two measurements for individual directional reconstructions. (c), (f), and (i) Statistical distributions of inter- and intra-HDs corresponding to the reconstructed 3D PUFs. (j) Box plot of HDs for stereoscopic 3D PUF reconstructed from independent X , Y , and Z directions. (k) Fusion-based reconstruction strategy integrating microtexture features from all three crystallographic directions of the same PUF. (l) Pairwise cross-correlation analyses and statistical HD distributions for fused 3D PUFs. (m) Statistical distributions of inter- and intra-HDs corresponding to the reconstructed 3D PUFs. (n) Box plot of HDs for fusion-reconstructed stereoscopic PUFs.

topology). Fused results (Figs. 5(l)–5(n)) confirm performance improvements: cross-correlation curves (Fig. 5(l)) exhibit higher overlap (correlation coefficients > 0.9), intra-HD remains concentrated around 0.1, and inter-HD distributes around 0.487. Figures S37 and S38 in the ESM demonstrate the process and results of constructing quaternary 3D PUFs through 3D reconstruction of microtexture images from the X, Y, and Z directions of the same PUF, which also exhibit this pattern. Figure 5(n) is a boxplot of HD for 3D stereoscopic PUFs reconstructed from binary/quaternary X/Y/Z IPFs, demonstrating that fused three-direction PUFs also maintain good stability and uniqueness. The stability of the 3D PUF obtained through 3D reconstruction was characterized in Figs. S39–S60 in the ESM. The results demonstrate that both the single-direction-based and the three-direction-fused reconstruction approaches exhibit excellent stability. In summary, 3D PUFs reconstructed from either single-direction or three-direction IPFs are suitable for use as PUFs in security applications.

While conventional EBSD-based 2D/3D PUFs leverage crystal orientation coloring to establish visually distinguishable physical entropy sources, their security mechanism fundamentally relies on stochastic image color distribution, which inherently suffers from vulnerability to optical spoofing attacks and entropy density limitations imposed by pixel resolution. To overcome these constraints, this work proposes a crystallographic encoding strategy. By quantitatively decoupling the spatial proportions of the {100}/{110}/{111} three-plane system and establishing statistical models, we achieve a dimensional elevation of security primitives—from “chromatic representation” to “crystallographic microtexture features”. The competitive occupancy ratios of these low-index planes directly correlate with intrinsic quantum attributes such as dislocation slip barriers and surface energy minima. Through this material-genome-directed extraction, physical unclonability transcends macroscopic morphological randomness, delving into the unpredictable atomic arrangements governed by Bragg diffraction, thereby erecting an insurmountable quantum-resistant shield against AI spoofing and physical cloning.

Figure 6 demonstrates the crystallographic encoding of polycrystalline diamond microtexture, where Figs. 6(a)–6(c) present EBSD-derived IPFs (IPF-X/IPF-Y/IPF-Z/IPF-C) for two independent tests on PUF₁ (Figs. 6(a) and 6(b)) and one test on PUF₂ (Fig. 6(c)), quantitatively extracting the frequency proportions of (100)/(110)/(111) planes (e.g., IPF-X (100) proportion: 20.55% → rounded to 21%); Figs. 6(d)–6(f) convert these proportions into 24-bit integer code chains sequenced as IPF-X → IPF-Y → IPF-Z → IPF-C (e.g., “212122-201920-291731-191617” encodes IPF-X:21%/21%/22%, IPF-Y:20%/19%/20%, IPF-Z:29%/17%/31%, IPF-C:19%/16%/17%), achieving extreme data compression; Fig. 6(g) validates repeatability via five repeated tests on one label, confirming crystal plane proportion stability; Fig. 6(h) outputs consistent encoding matrices across all five tests (e.g., recurring sequence “161619-171717-211822-191613”), rigorously proving encoding rule rigidity and noise immunity, thereby establishing a reproducible 24-bit digital fingerprint for multidimensional texture characterization.

3 Conclusion

In summary, this study pioneers a triple collaborative encryption framework by leveraging the crystallographic disorder of polycrystalline diamond. It achieves microtexture-based fingerprint

encoding by extracting the proportional distributions of {100}/{110}/{111} crystal planes through IPF-X/IPF-Y/IPF-Z maps, combined with multi-base (2/4/8/16/32) conversion of IPF maps to generate high-entropy keys resistant to brute-force attacks. The 3D reconstruction of IPF data establishes a tamper-proof spatial topology, ensuring fingerprint integrity even in extreme environments. Breakthrough flexible diamond substrate technology extends its application beyond rigid carriers—maintaining diamond’s ultimate durability while enabling conformal integration with wearable devices and curved surfaces. This system uses the material genome as its security foundation, leveraging atomic-level stochastic grain growth to prevent replication at zero additional cost. It supports cross-scale authentication from macroscopic curved screens to quantum chips, establishing a tamper-proof standard for aerospace components, pharmaceutical packaging, and hardware root of trust. Future work will focus on miniaturized deployment for machine vision and coupled applications of quantum dot-optical cryptographic protocols.

4 Experimental section

4.1 CVD growth of rigid diamond film

Heteroepitaxial growth of rigid polycrystalline diamond film on a silicon substrate involves two steps: substrate pretreatment and CVD diamond growth. First, a 2-inch silicon substrate undergoes meticulous mechanical polishing to deliberately introduce a high density of uniformly distributed nucleation sites. Following this critical pretreatment, the substrate is placed in a microwave plasma chemical vapor deposition (MPCVD) system for growth under the following parameters: 3850 W microwave power, 135 Torr chamber pressure, 850 °C temperature, 190 sccm H₂ flow, 10 sccm CH₄ flow, and a 300-hour duration.

4.2 CVD growth of flexible diamond film

Heteroepitaxial growth of flexible diamond film on a silicon substrate comprises three steps: substrate pretreatment, diamond seeding, and CVD diamond growth. First, silicon surface pretreatment is performed using hydrogen plasma: a 1-inch silicon wafer is placed in an MPCVD system and treated at 1400 W power, 40 Torr chamber pressure, and 300 sccm H₂ flow for 10 min. Diamond seeding involves mixing, dispersion, and centrifugation steps. Diamond seeds (5 nm size) are mixed with dimethyl sulfoxide (DMSO), anhydrous ethanol, and acetone at a mass ratio of 1:5000:250:250. The mixture is ultrasonicated for 12 h for dispersion, followed by centrifugation at 1000 rpm for 20 min to separate impurities. The resulting suspension is then spin-coated onto the silicon wafer (parameters: 500 rpm for 10 s while dispensing 10 drops, then increased to 4500 rpm for 120 s). The seeded wafer is transferred to the MPCVD system for diamond film growth under the following conditions: 3850 W microwave power, 135 Torr chamber pressure, 850 °C temperature, 185 sccm H₂ flow, 15 sccm CH₄ flow, and a 40-minute growth duration. Specifically, the self-supported flexible polycrystalline diamond films were obtained using two approaches: (1) mechanical peeling with adhesive tape, and (2) selective chemical etching of the silicon substrate using NaOH solution. Both methods successfully produced free-standing flexible diamond films suitable for subsequent characterization and device-related evaluation.

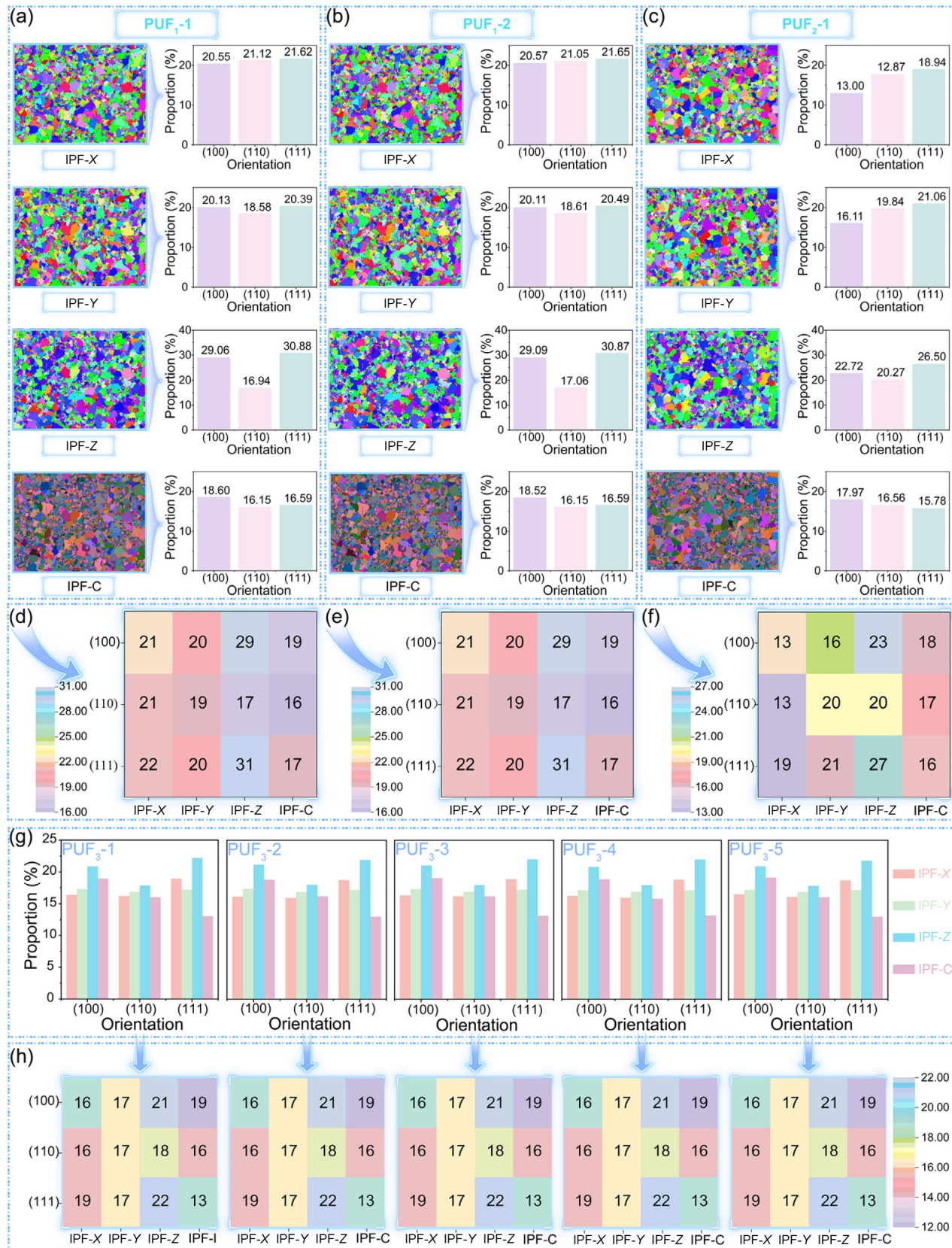


Figure 6 Crystallographic encoding based on lattice-plane population statistics. (a)–(c) Extracted proportions of (100), (110), and (111) lattice planes from IPF-X, IPF-Y, IPF-Z, and IPF-C maps of two measurements of PUF₁ and one measurement of PUF₂. (d)–(f) Corresponding crystallographic encoding results derived from the plane proportion statistics in (a)–(c). (g) Plane proportion statistics extracted from five independent EBSD measurement of the same PUF label. (h) Crystallographic encoding results demonstrating reproducibility across repeated measurements.

4.3 EBSD characterization

EBSD analysis was conducted using an Oxford Instruments Symmetry EBSD detector integrated with a Zeiss field-emission scanning electron microscope (FESEM). The sample was prepared by ion beam polishing (argon ion energy: 4 keV, incident angle: 4°, duration: 1 h) to achieve a stress-free surface. The measurement parameters were configured as follows: accelerating voltage of 20 kV, working distance of 14.5 mm, stage tilt angle of 70°, scan step size of 800 nm (matched to diamond grain dimensions), single-point acquisition time of 50 ms, and Hough resolution parameter of 70. To ensure reliable relocation of identical microscopic regions during repeated EBSD measurements, lithographically defined metallic fiducial markers were fabricated on the sample surface prior to characterization. These alignment markers enabled accurate repositioning of the same microtexture region during successive EBSD acquisitions, thereby ensuring the repeatability analysis presented in the manuscript.

Electronic Supplementary Material: Supplementary material (complete experimental data of the multidimensional PUF encryption system based on polycrystalline diamond microtexture; 2D encoding schemes ranging from binary to duotrigesimal are implemented relying on four types of IPF orientation maps (X, Y, Z, and C), and the encryption performance of the PUFs is verified via entropy, Hamming distance, cross-correlation and other metrics; two 3D reconstruction workflows (single-direction reconstruction and three-direction fusion reconstruction) are demonstrated step-by-step; combined with the results of repeated measurements, the excellent uniqueness and reproducibility of both 2D and 3D diamond-based PUFs are validated) is available in the online version of this article at <https://doi.org/10.26599/NR.2026.94908855>.

Data availability

All data needed to support the conclusions in the paper are presented in the manuscript and the Electronic Supplementary Material. Additional data related to this paper may be requested from the corresponding author upon request.

Acknowledgements

This work was financially supported by the Foundation of National Key Laboratory of Plasma Physics (No. 6142A04240204), the National Natural Science Foundation of China (Nos. U22A2077 and U25A20192), Postgraduate Education Reform and Quality Improvement Project of Henan Province (No. YJS2025GZZ04), Joint Fund of Henan Province Science and Technology R&D Program (Nos. 245200810005 and 245200810091), Fundamental Research Fund of Henan Academy of Sciences (No. 20250627005), and High-level Talent Research Start-up Project Funding of Henan Academy of Sciences (No. 241827231).

Declaration of competing interest

All the contributing authors report no conflict of interests in this work.

Author contribution statement

Z. F. Z.: Data curation, project administration, validation, writing

manuscript, experimental design. X. Y.: Validation, experimental design. C. N. L.: Data curation, project administration, writing manuscript. J. H. Z.: Project administration, validation, experimental design. L. D.: Project administration, funding acquisition, writing manuscript. C. X. S.: Funding acquisition, writing manuscript. All the authors have approved the final manuscript.

Use of AI statement

None.

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