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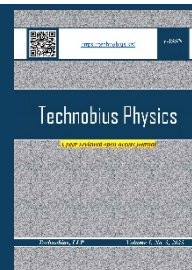
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CONTENTS

Title and Authors	Category	No.
Comprehensive Overview of X-Ray Diffraction: Principles, Techniques, and Applications in Material Science <i>Hersh F Mahmood, Soran Abdrahman Ahmad, Masood Abu-Bakr</i>	<i>Condensed Matter Physics</i>	0035
Correlation between surface nanomorphology and charge density waves in 1T-TaS ₂ <i>Anton Shuravin</i>	<i>General Physics Condensed Matter Physics</i>	0036
Quantum effects in weak gravitational fields: towards tabletop tests of quantum gravity <i>Elmira Sayabekova</i>	<i>General Physics</i>	0037
Numerical framework for simulating quantum spacetime fluctuations with prescribed spectra <i>Do-Yoon Lee, Gye-Tai Park</i>	<i>General Physics</i>	0038
Thickness- and gate-tunable ferromagnetism in low-dimensional Fe ₃ GeTe ₂ nanoflakes <i>Zhang Wei</i>	<i>General Physics Condensed Matter Physics</i>	0039



Review

Comprehensive Overview of X-Ray Diffraction: Principles, Techniques, and Applications in Material Science

Hersh F Mahmood^{1,*}, Soran Abdrahman Ahamd², Masood Abu-Bakr¹.

¹Civil Engineering Department, University of Halabja, Halabja, Kurdistan Region, Iraq

²Civil Engineering Department, College of Engineering, University of Sulaimani, Sulaimani, Kurdistan Region, Iraq

*Corresponding author: hersh.fage@uoh.edu.iq

Abstract. This paper provides an overview of XRD, including its principles, instrumentation, data analysis, and applications. While visual characteristics can aid in identifying certain minerals, powder XRD remains the most reliable and accurate method for phase identification and structural analysis. Beyond crystallography, XRD offers valuable insights into the short- and intermediate-range structures of amorphous materials such as glasses, revealing its broader relevance in emerging technologies. It is widely used for analyzing powders, solids, thin films, and nanomaterial. XRD is often combined with techniques like SEM, TEM, PCS, EBSD, SPM, DLS, ND, and SAED to enhance material characterization. The paper covers fundamental principles such as Bragg's Law and X-ray interaction with crystal lattices, as well as advancements in XRD instrumentation, including X-ray sources, diffractometer, and detectors, reflecting the rapid scientific progress in XRD technology.

Keywords: X-ray, diffraction, material science, non-destructive analysis, microstructure characterization.

1. Introduction

X-ray diffraction (XRD) is a powerful analytical technique used to determine the molecular structure of crystalline materials by measuring the diffraction of X-rays through a sample. The resulting interference patterns provide information about the lattice structure, allowing researchers to analyze parameters such as unit cell dimensions, crystal symmetry, strain, and defects. The discovery of X-rays by W.C. Röntgen in 1895 [1] marked the beginning of this field. In 1912, Max von Laue proposed that X-rays have wavelengths comparable to interatomic distances in crystals. Acting on his idea, Walter Friedrich and Paul Knipping conducted the first X-ray diffraction experiment on crystals [2]. In 1913, William Henry Bragg and his son William Lawrence Bragg discovered the crystal structure of sodium chloride (NaCl), laying the foundation for X-ray crystallography. The Braggs' work explained how cleavage faces of crystals reflect X-rays at specific angles—now described by Bragg's Law. Shortly after, in 1916, P. Debye and P. Scherrer developed methods to analyze polycrystalline materials [2]. XRD instruments have evolved since Karl Weissenberg introduced the Weissenberg camera in the 1920s, although the fundamental principles remain largely unchanged. Significant advancements have been made with the integration of minicomputers for instrument control, data acquisition, and processing [3].

This paper provides a comprehensive overview of XRD techniques, including their historical development, instrumentation, work procedures, sample preparation, and broad applications. Among various XRD techniques, powder X-ray diffraction (PXRD) is particularly notable for its ability to simultaneously characterize both precursor and final products, providing a complete qualitative assessment of microstructural behavior [4]. When the Bragg angle is unknown for a new crystalline

material, two primary techniques are used to generate diffraction patterns: the Laue method and the rotation method. The Laue method, developed by Max von Laue, involves exposing a stationary single crystal to a broad, white spectrum of X-rays. This allows for rapid determination of crystal symmetry and orientation by capturing a comprehensive snapshot of all diffraction directions. While useful for studying highly symmetric or complex structures, its diffraction patterns often contain overlapping spots, complicating interpretation. It is mainly used for qualitative analysis when the exact wavelength of the X-rays is not well known [5].

In contrast, the rotation method – also known as the oscillation or precession method – involves rotating the crystal in a monochromatic X-ray beam of known wavelength. This technique collects diffraction data across multiple angles and is used in both single-crystal and powder diffraction studies. For powdered samples, it is referred to as powder diffraction; for intact crystals, it is called single-crystal diffraction. Both methods rely on measuring the intensity of diffracted X-rays as the sample, tube, or detector moves to vary the diffraction angle (2θ), the angle between the incident and diffracted beams. These measurements are critical for structural characterization. The diffraction angle provides insights into the interplanar spacing (d-spacing) of the crystal lattice, essential for structural determination using Bragg's Law. By analyzing the positions, intensities, and shapes of diffraction peaks, researchers can derive key structural details such as crystallite size, chemical bonding, and lattice distortions – parameters that directly influence the physical properties and potential applications of materials in fields such as chemistry, materials science, and nanotechnology. The atomic arrangement within a crystal can also be determined by reconstructing the observed diffraction pattern. Symmetry, lattice constants, and defect structures can be identified with high precision. Tools like the Renninger diagram – which plots X-ray reflection intensity against the angle of incidence – further assist in structural analysis. For example, identifying a single forbidden reflection can help determine specific isomeric forms and subtle atomic configurations [6].

Modern XRD techniques have expanded these capabilities. Grazing Incidence XRD (GIXRD), a non-destructive method, is especially suited for thin films and coatings, allowing analysis without damaging the sample. It also enables direct assessment of film density through grazing incidence angle-dependent scattering intensity [7]. High-Resolution XRD (HRXRD) employs highly monochromatic beams and optics with extremely low angular divergence to achieve sub-angstrom resolution. It is particularly effective for measuring strain, composition, thickness, and crystalline quality in epitaxial films and heterostructures [8]. HRXRD has been used to confirm epitaxial growth and detect internal grain boundaries in crystals grown by various techniques using multicrystal diffractometer [9]. Accurate simulations of reciprocal space maps (RSMs), accounting for the effects of mirrors, monochromators, analyzers, and slits, have shown strong agreement with experimental data, as demonstrated with a perfect Si(110) crystal [10]. Furthermore, combined real and reciprocal space X-ray mapping techniques are now widely employed to investigate the epitaxial growth of semiconductors [11]. The versatility, precision, and non-destructive nature of XRD make it indispensable in both scientific research and industrial applications, including material development, quality control, and microstructure analysis. The technique continues to evolve, driving innovation across multiple fields. The XRD technique is widely used for microstructure measurement, testing, and in-depth research investigations. The instrument is shown in Figure 1.

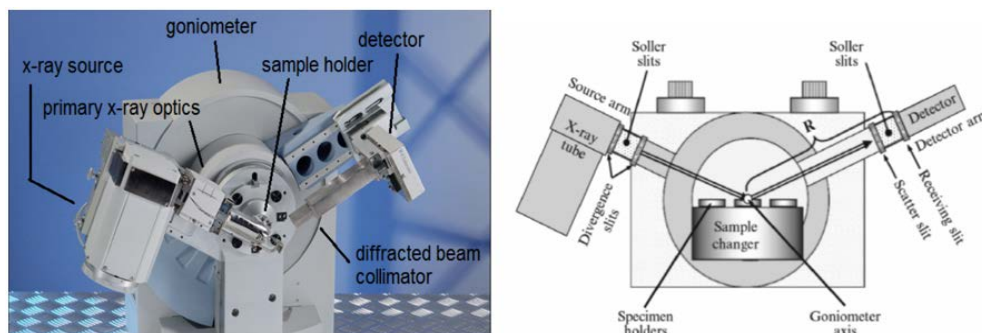


Figure 1 – XRD instrument for microstructural analysis and research applications

2. Methods

This review was conducted using a structured and systematic approach to ensure comprehensive coverage of the scientific literature related to XRD, its principles, instrumentation, and applications in material science. The methodology comprised three main stages: literature search, study selection, and data extraction and synthesis.

2.1 Literature Search Strategy

A comprehensive literature search was undertaken to identify relevant studies published between 2000 and 2025. The search was performed across several major scientific databases, including Scopus, Web of Science, ScienceDirect, SpringerLink, and IEEE Xplore, which are recognized for their extensive coverage of peer-reviewed publications in physics and materials science. To supplement this search, additional sources such as Google Scholar and ResearchGate were examined for grey literature and conference proceedings not indexed in the aforementioned databases.

The search strategy employed a combination of keywords and Boolean operators to maximize retrieval of relevant studies. Search terms included "X-ray diffraction" OR "XRD", "powder X-ray diffraction" AND "material characterization", "GIXRD" OR "HRXRD" AND "applications", and "X-ray diffraction" AND "crystal structure analysis". Filters were applied to restrict results to publications in the English language and peer-reviewed sources only. All identified records were exported to Mendeley reference management software, where duplicate entries were removed.

2.2 Inclusion and Exclusion criteria

Studies were screened based on predefined criteria to ensure that only high-quality and relevant literature was included in this review. The inclusion criteria were as follows:

- Articles published in peer-reviewed journals, conference proceedings, or authoritative book chapters focusing on XRD principles, methodology, or applications in materials science.
- Research presenting experimental or theoretical investigations, technological advancements, or combined analytical approaches involving XRD (e.g., integration with SEM, TEM, or synchrotron techniques).
- Studies providing sufficient detail regarding experimental setup, data acquisition, and analysis procedures.

Conversely, publications were excluded if they met one or more of the following conditions:

- Non-English language publications.
- Non-peer-reviewed articles, opinion pieces, or editorials lacking scientific rigor.
- Studies focusing exclusively on medical imaging or other X-ray-based methods unrelated to diffraction analysis.
- Duplicates or sources without methodological or analytical depth.

2.3 Data Extraction and Synthesis

Following the screening process, a total of 112 studies were selected for detailed review. Relevant information was extracted from each study using a structured template, capturing bibliographic details (authors, publication year, and journal source), type of XRD technique investigated (PXRD, GIXRD, HRXRD, or synchrotron-based methods), study objectives, experimental conditions, sample characteristics, and reported findings.

The extracted data were analyzed qualitatively to identify recurring themes, methodological advancements, and application trends in XRD research. Comparative evaluation was conducted to highlight similarities and differences among studies, particularly in relation to instrumentation design, data acquisition strategies, and interpretation of diffraction patterns. The findings were then synthesized into thematic categories representing the historical development, theoretical principles, technical progress, and modern applications of XRD. This approach ensured a coherent narrative that

reflects the current state of knowledge while identifying research gaps and directions for future investigations.

3-N. X-Ray Diffractometer: Components, Mechanism, and Applications

XRD is a fundamental analytical technique used to investigate the atomic and molecular structure of crystalline materials. This chapter provides an in-depth examination of the XRD device components, the principles underlying its operation, variations in experimental geometry, and its diverse applications. The information is synthesized from various studies [2], [3], [7], [8], [12], [13], [14], [15], [16], highlighting the current state of knowledge and identifying critical advancements in the field.

3.1 Components of the XRD Device

The standard X-ray diffractometer consists of three primary components: the X-ray source (tube), the sample holder, and the X-ray detector. Each element performs a distinct function that is essential to producing high-quality diffraction data.

The X-ray tube generates X-rays through thermionic emission. Electrons emitted from a heated tungsten filament are accelerated under high voltage toward a target material, typically copper or molybdenum. When the electron beam collides with the target, inner-shell electrons are ejected, creating vacancies filled by outer-shell electrons. The transition releases energy in the form of characteristic X-rays whose wavelengths are specific to the target element (Figure 2). These X-rays are directed toward the sample for analysis.

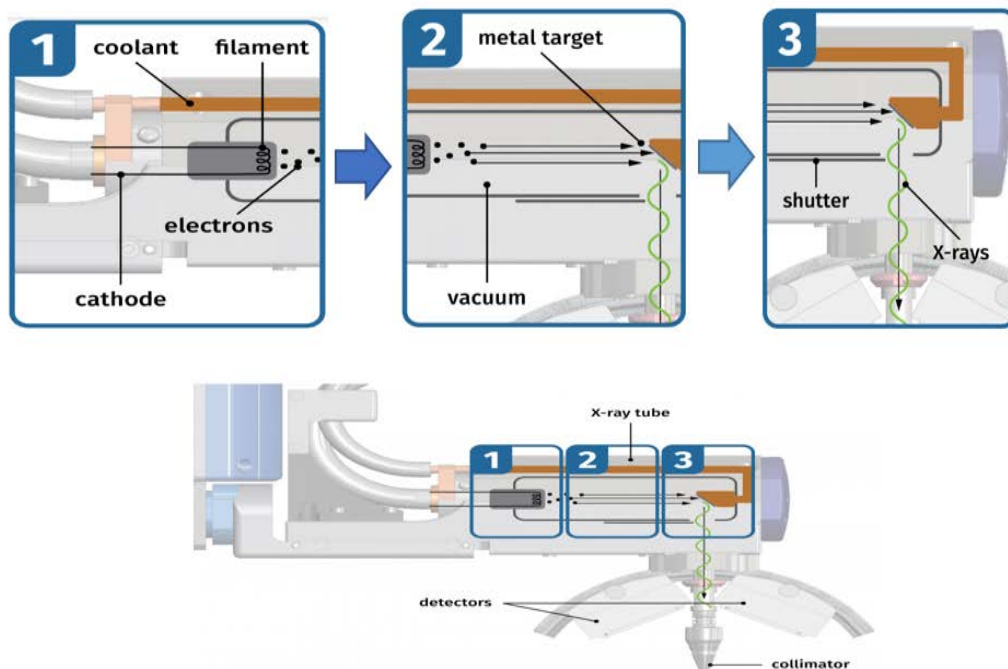


Figure 2 – Mechanism of X-ray generation

The sample holder positions the specimen within the beam path. Its design must minimize background scattering and ensure precise alignment, as even minor deviations can affect diffraction patterns. The detector collects the diffracted beams, converting X-ray intensity into electronic signals that are subsequently processed to generate a diffraction pattern. This pattern reveals information about crystal symmetry, atomic arrangement, and interplanar spacings [2], [4].

3.2 Experimental geometry and reflection mode

In a typical XRD experiment operating in reflection mode, the X-ray source remains fixed while the sample rotates relative to the incident beam. This rotation allows the beam to probe different crystallographic planes of the material. Simultaneously, the detector rotates at twice the angle of the sample (2θ geometry) to capture diffracted rays accurately. This configuration ensures reliable recording of diffraction peaks and facilitates calculation of interplanar spacing using Bragg's law [3], [7]:

$$n\lambda = 2d \sin \theta \quad (1)$$

Where n is an integer, λ is the X-ray wavelength, d is the interplanar spacing, and θ is the diffraction angle. The resulting diffraction peaks provide quantitative information on phase composition, crystallinity, and structural defects (Figure 3).

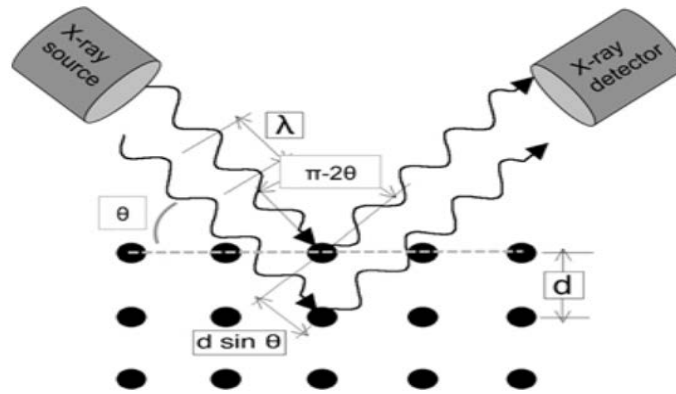


Figure 3 – Schematic illustration of the experimental geometry

Advanced geometries, including GIXRD and HRXRD, have been developed to enhance analytical sensitivity. GIXRD utilizes a shallow incident angle, improving the characterization of thin films and surface layers without damaging the sample [26]. HRXRD employs monochromatic beams and high-precision optics, enabling sub-arcsecond angular resolution crucial for studying epitaxial films and semiconductor interfaces [17] (Figures 4 and 5).

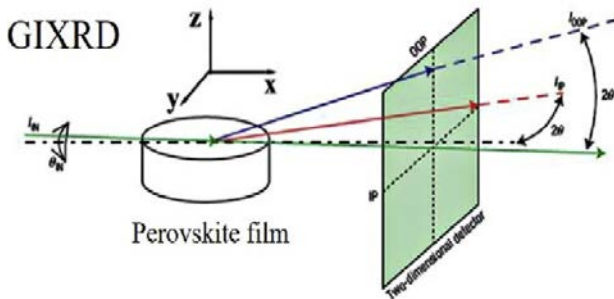


Figure 4 – GIXRD experimental setup [17]

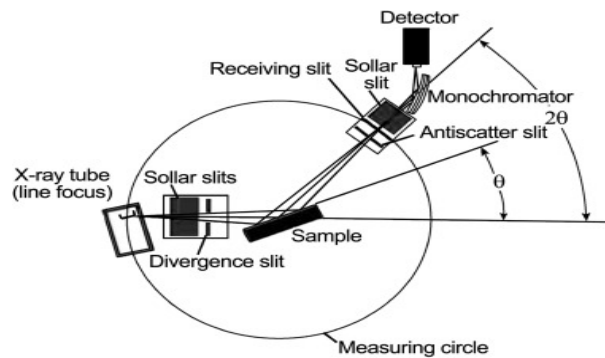


Figure 5 – Schematic diagram of HRXRD setup for epitaxial layer and interface analysis [17]

Table 1 summarizes the primary features and applications of PXRD, GIXRD, and HRXRD, illustrating their complementarity in material characterization.

Table 1 – Comparison of XRD techniques, their applications, and geometrical configurations

#	Technique	Purpose	Geometry Highlights
1	PXRD	Bulk crystal structure from powders	θ - 2θ scan; random orientation
2	GIXRD	Thin film analysis	Small incident angle; surface-sensitive
3	HRXRD	High-resolution strain and defect mapping	Optics-enhanced; precise angular resolution

3.3 Mechanism of XRD analysis

The principle of XRD is based on constructive interference of monochromatic X-rays scattered by periodic crystal planes. Millions of crystallites within a powdered sample contribute simultaneously to the observed diffraction pattern, assuming a random orientation distribution. The resulting intensities depend on crystallite size, defects, and orientation [7].

Mineral identification using XRD typically involves two steps: (i) peak matching between the experimental pattern and reference databases, and (ii) comparison of observed diffraction angles (2θ) to standard values [8]. However, amorphous phases, preferred orientation, and sample imperfections can complicate data interpretation, requiring careful calibration and sometimes complementary analytical methods.

Recent studies demonstrate that instrument geometry and crystallite orientation strongly affect peak intensities. For example, Fewster [7] highlighted deviations in predicted intensity values when comparing kinematical and dynamical scattering theories, particularly for micrometer-sized crystallites. Additionally, thermal effects during X-ray generation can cause intensity variations exceeding 15% [16], emphasizing the importance of controlled experimental conditions.

3.4 Applications across scientific disciplines

XRD has become indispensable in materials research, pharmaceuticals, geology, and even planetary science. The CheMin XRD instrument aboard NASA's Mars Science Laboratory successfully identified clay minerals and amorphous phases on Mars' surface, demonstrating the technique's robustness in extraterrestrial environments [11], [12], [18].

In pharmaceutical studies, XRD provides critical insights into polymorphic forms of drug compounds, essential for drug stability and efficacy [13]. Industrially, fully automated XRD systems optimize production processes in mining, cement, and superconductor manufacturing by delivering rapid and reliable phase identification [14]. Furthermore, synchrotron-based high-resolution diffraction measurements offer unparalleled sensitivity in detecting strain states in advanced composite conductors [14], [4].

The growing interest in nanomaterials and hybrid polymers has expanded XRD applications. As reported in [15], [16], [17] temperature-dependent XRD spectra reveal changes in nanoparticle size and morphology, while combined XRD-SEM analyses elucidate structural modifications in graphene oxide-based composites, enhancing understanding of their electrical and mechanical properties.

3.5 Sample preparation and its influence on data quality

Proper sample preparation is critical for reliable diffraction data. Finely ground powders ($<44\ \mu\text{m}$) ensure random crystallite orientation, improving peak sharpness and intensity. Coarse powders, in contrast, produce broader, less intense peaks, complicating structural interpretation (Figure 6). As demonstrated in [4], sample homogeneity, moisture content, and contamination can significantly degrade signal quality.

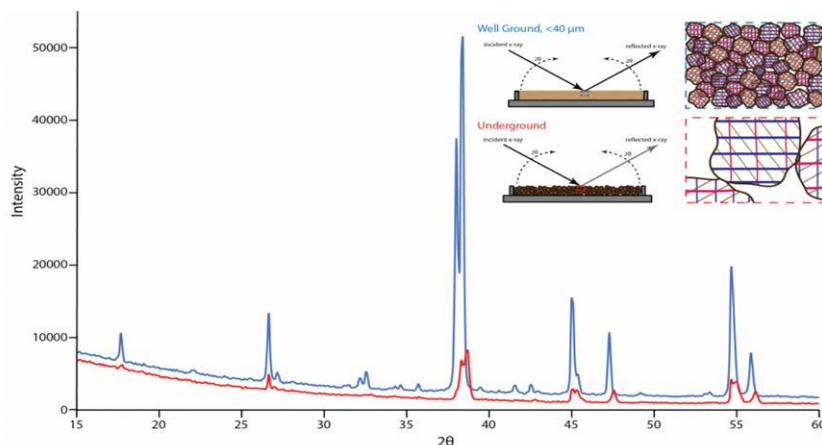


Figure 6 – Diffraction patterns of two samples with different grain sizes

Preferred orientation effects are particularly problematic in metals and polymers, where crystallites align due to manufacturing processes. Misalignment in the sample holder can suppress certain reflections, leading to incomplete data. Rotating the specimen by 90° during measurement, as recommended in [4], can mitigate these artifacts, producing a diffraction pattern representative of the bulk material (Figure 7).

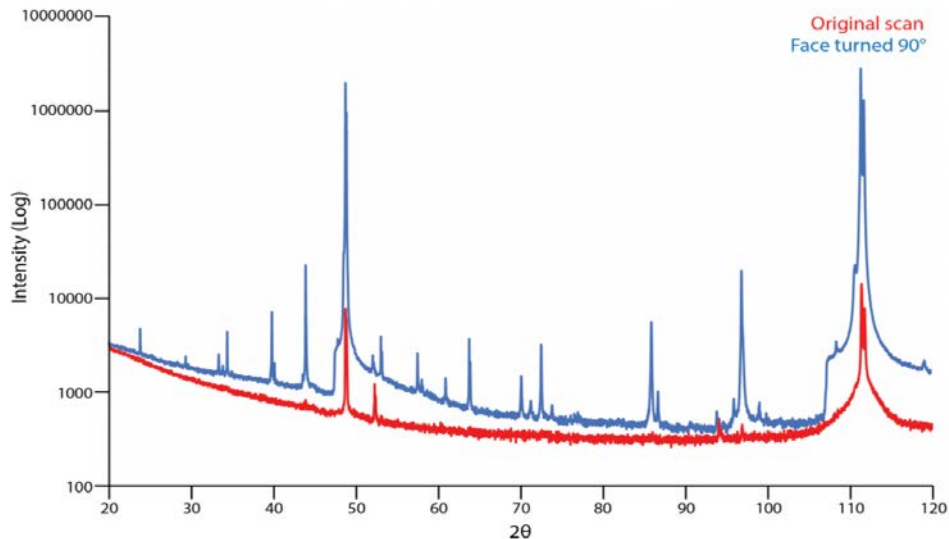


Figure 7 – Initial orientation showing many undetected peaks due to a 90° rotation of the sample surface

3.6 Synthesis of Findings

The reviewed studies collectively demonstrate that the accuracy and reliability of XRD measurements depend on multiple factors: instrument design, geometry configuration, and sample preparation techniques. Technological advances such as GIXRD, HRXRD, and synchrotron sources have expanded the resolution and sensitivity of XRD analyses, enabling nanoscale and in-situ studies across diverse scientific fields. However, achieving reproducible results still requires careful control of experimental conditions, meticulous sample handling, and standardized analytical protocols.

4. Discussion

The analysis of the reviewed literature confirms that XRD remains one of the most powerful and widely utilized analytical techniques for investigating the structural properties of crystalline materials. The reviewed studies consistently demonstrate that PXRD provides a highly reliable and reproducible approach for phase identification and structural characterization, surpassing other macroscopic identification methods such as visual inspection of mineral color or crystal morphology. PXRD is particularly indispensable for analyzing complex multi-phase systems and amorphous materials, where conventional identification approaches are insufficient.

The findings highlight that XRD techniques extend beyond simple phase identification, providing valuable insights into short- and intermediate-range atomic structures, especially in non-crystalline materials such as glasses. This capability opens avenues for understanding structural disorder and its influence on the physical properties of advanced materials, thereby driving innovations in fields such as photonics, catalysis, and nanotechnology. Moreover, XRD enables simultaneous evaluation of lattice parameters, crystallite size, strain, and defect distributions, establishing its role as a cornerstone technique for correlating structural characteristics with functional performance.

The review also indicates that XRD applications have expanded significantly across diverse domains, including pharmaceutical sciences, archaeology, electronics, and material engineering,

where non-destructive, high-precision analysis is critical. In these fields, XRD provides essential information on the composition, crystallinity, and stability of substances without altering their intrinsic properties, making it invaluable for both research and industrial quality control.

Recent technological advancements—such as high-resolution XRD, grazing-incidence XRD (GIXRD), and synchrotron-based diffraction methods—have greatly enhanced analytical precision and sensitivity. These developments enable the detection of subtle structural features such as strain gradients in thin films, epitaxial layer mismatches in semiconductors, and nanoscale heterogeneities in composite materials. The integration of XRD with complementary techniques (e.g., SEM, TEM, and spectroscopy) further strengthens its potential for multi-modal characterization.

The reviewed literature underscores that XRD remains a fundamental and irreplaceable tool in modern materials science, playing a pivotal role in understanding the relationship between structure and material properties. Its non-destructive nature, high accuracy, and adaptability to different sample types make it essential for the design, development, and optimization of new materials. As industries increasingly move towards high-performance functional materials, demand for more advanced, rapid, and automated XRD solutions is expected to grow, particularly in high-throughput research environments.

Based on the synthesis of current knowledge, several promising research directions can be outlined:

- Development of in-situ and operando XRD techniques to monitor structural transformations of materials under real-world conditions (e.g., high temperature, high pressure, electrochemical cycling).

- Improvement of spatially resolved XRD methods for nanoscale structural mapping, particularly relevant for next-generation electronics and nanomaterials.

- Advancements in data processing and machine learning algorithms for automated phase identification, noise reduction, and quantitative analysis of complex diffraction patterns.

- Integration of XRD with complementary multi-scale characterization tools, enabling correlative studies that bridge atomic-scale and macroscopic material behavior.

- Expansion of XRD applications to emerging materials, such as perovskite solar cells, 2D materials, and hybrid organic–inorganic frameworks, where understanding defect structures and phase stability is crucial.

Overall, XRD continues to be an indispensable technique for the structural elucidation and optimization of functional materials. Ongoing methodological improvements, coupled with enhanced data analysis capabilities, are expected to broaden its applicability and accelerate material discovery in the coming decades.

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Information about authors:

Hersh F Mahmood – PhD, Lecture, Civil Engineering Department, University of Halabja, Halabja, Kurdistan region, Iraq, hersh.faqe@uoh.edu.iq
Soran Abdrahman Ahmad – MSc, Lecture, Civil Engineering Department, University of Sulaimani, Sulaimani, Kurdistan region, Iraq, soran.abdrahman@univsul.edu.iq
Masood Abu-Bakr – MSc, Lecture, Civil Engineering Department, University of Halabja, Halabja, Kurdistan region, Iraq, masoud.mohammed@uoh.edu.iq

Author Contributions:

Hersh F Mahmood – concept, methodology, interpretation, editing.
Soran Abdrahman Ahmad – modeling, analysis, visualization, drafting;
Masood Abu-Bakr – resources, data collection, testing, funding acquisition.

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Correlation between surface nanomorphology and charge density waves in 1T-TaS₂

 Anton Shuravin*

Institute for Nanomaterials, Advanced Technologies and Innovation, Technical University of Liberec, Liberec, Czech Republic

*Correspondence: antony.shuravin@gmail.com

Abstract. This study investigates the structural and electronic properties of 1T-TaS₂ using scanning tunneling microscopy (STM) and complementary Fourier analysis. The objective was to correlate surface morphology with the emergence of commensurate charge density wave (CDW) order and to quantify the periodicities governing its modulation. High-resolution STM imaging revealed both the atomic lattice and the superimposed CDW, with measured lattice constant of 0.343 ± 0.02 nm and CDW periodicities of 1.1 ± 0.05 nm and 2.0 ± 0.05 nm. Fourier transforms confirmed reciprocal vectors of 2.9 ± 0.1 nm⁻¹ for the lattice and $0.5\text{--}0.9 \pm 0.1$ nm⁻¹ for the CDW, rotated by approximately 30° with respect to the atomic lattice, consistent with a commensurate $\sqrt{13} \times \sqrt{13}$ reconstruction. Surface roughness characterization showed root-mean-square variations of 3.5 ± 0.2 nm and terrace widths of only 25–40 nm, reflecting the brittle nature of the crystal and highlighting constraints for achieving atomically stable imaging. Bias-dependent measurements demonstrated contrast inversion between filled and empty states, providing direct evidence of the electronic origin of the CDW. These results confirm the robustness of CDW ordering in 1T-TaS₂, address the research objective of linking morphology with electronic superstructures, and highlight both the opportunities and challenges of using this material as a platform for studying correlated electron phenomena in low-dimensional solids.

Keywords: scanning tunneling microscopy, charge density waves, surface roughness, nanomorphology, Fourier analysis, commensurate superstructure.

1. Introduction

Charge density waves (CDWs) are collective electronic phenomena where conduction electrons couple strongly with the underlying lattice, producing a periodic modulation of both charge density and atomic positions [1]. The concept originates from Rudolf Peierls [2], who first explained how, in a one-dimensional crystal, periodic lattice distortions can open band gaps at multiples of:

$$k = \frac{\pi}{a} \quad (1)$$

in the electronic dispersion $E(k)$. In the ground state, electrons occupy states up to the Fermi level at

$$k_F = \pm \frac{\pi}{2a} \quad (2)$$

lowering the electronic energy. This distortion becomes energetically favorable if the electronic energy gain outweighs the elastic cost, below a characteristic Peierls transition temperature. As a result, the CDW state can drive a transition from a metallic to a semiconducting or insulating phase. Although Peierls' mechanism is most direct in one dimension, CDWs have also been observed in two- and three-dimensional materials, where the theoretical description is more complex but no less significant [2].

Transition-metal dichalcogenides (TMDs) provide a particularly rich platform for investigating CDWs due to their layered structures and weak interlayer van der Waals bonding. Among them, 1T-TaS₂ has attracted sustained attention as a model system [3]. In its 1T polytype,

each tantalum layer is sandwiched between sulfur layers, producing a quasi-two-dimensional structure that readily exhibits CDW instabilities. The system undergoes multiple phase transitions: below 183 K, a fully commensurate CDW forms; between 183 K and 353 K, a nearly commensurate phase with mixed commensurate and incommensurate domains emerges; and above 353 K, the material stabilizes an incommensurate CDW phase. In real-space imaging, these modulations appear as a $\sqrt{13} \times \sqrt{13}$ “star-of-David” superlattice rotated by 30° relative to the atomic lattice. Scanning tunneling microscopy (STM) is uniquely capable of resolving this superlattice by directly probing the electronic density of states superimposed on the atomic lattice.

Recent experimental advances have expanded the understanding of CDWs in TaS₂ and related TMDs. [4] demonstrated nanoscale coexistence of commensurate and nearly commensurate CDWs using low-temperature STM. [5] highlighted the interplay between CDW order and Mott insulating behavior. [6] revealed metastable hidden CDW states induced by ultrafast optical pulses, opening pathways to switchable phases. [7] showed strain-induced tuning of CDW periodicity and stability, emphasizing the sensitivity of CDW order to external perturbations. More recently, [8] reported interlayer-stacking-driven switching between Mott- and band-insulating states in bulk TaS₂, while [9] observed proximity-induced CDW order in graphene/TaS₂ heterostructures with a concurrent reduction of the Mott gap. Thermal stabilization of hidden metallic CDW states has also been achieved by quenching [10], and epitaxial growth has enabled spiral TaS₂ structures with tunable electron correlations. Furthermore, STM studies by [11] revealed intradomain chirality in the nearly commensurate phase, while [12] mapped atomistic domain-wall networks forming a honeycomb lattice of metallic states. Collectively, these works underscore the robustness and tunability of CDWs in TaS₂, as well as their intimate connection to correlated electron phenomena.

Despite these advances, key questions remain. In particular, the correlation between surface morphology—including roughness, terrace width, and step density—and the visibility and stability of CDW order remains underexplored. While prior studies have largely focused either on electronic structure or on phase transitions, few have systematically integrated roughness quantification, reciprocal-space analysis, and bias-dependent STM imaging. This gap limits the ability to disentangle intrinsic CDW features from surface-induced artifacts.

We hypothesize that a combined methodology integrating topographic roughness analysis, Fourier transform mapping of periodicities, and bias-dependent STM contrast can establish a direct link between the surface morphology of TaS₂ and the stability of its CDW ordering.

The objective of this study is therefore to: (i) characterize the surface nanomorphology of 1T-TaS₂, (ii) resolve both atomic and CDW periodicities in real and reciprocal space, and (iii) determine how surface roughness and terrace size influence the stability and observability of CDW superstructures. By uniting structural and electronic perspectives, this work provides a comprehensive experimental framework for understanding collective electronic phenomena in layered dichalcogenides.

2. Methods

The choice of 1T-TaS₂ as the object of investigation is motivated by its layered crystal structure and the presence of a commensurate CDW state at low temperatures, which make it a prototypical system for studying collective electronic phenomena in low-dimensional solids. The material is also known to exhibit a Mott–Hubbard insulating phase arising from strong electron–electron correlations, rendering it a rare example where CDW order and Mott physics coexist in a single compound. This duality places 1T-TaS₂ at the center of modern solid-state research, as it enables direct exploration of the interplay between lattice instabilities, electron correlations, and low-dimensional confinement. Furthermore, its layered van der Waals nature facilitates preparation of atomically clean surfaces for STM, while also making the compound attractive for potential applications in nanoscale electronic and optoelectronic devices.

Experiments were conducted using a STM in order to resolve the surface electronic structure of layered transition-metal dichalcogenides. The procedure followed a well-established sequence aimed at ensuring tip stability, surface cleanliness, and high-resolution imaging down to the atomic scale. All measurements were performed at room temperature under ultrahigh vacuum (UHV) conditions, unless otherwise specified.

A mechanically cut Pt–Ir tip was prepared and tested on highly oriented pyrolytic graphite (HOPG), a standard calibration substrate widely used due to its atomically flat terraces and easily resolvable hexagonal lattice. Atomic resolution of the HOPG surface was required as a criterion of tip sharpness and stability. The test scan was performed at a sample bias of 50 mV and a tunneling set-point current of 1 nA, conditions optimized for the visualization of individual carbon atoms on the HOPG basal plane [13].

Following tip verification, the substrate was replaced by the TaS₂ crystal, cleaved in situ to expose a clean surface. The initial approach was performed with an image size of ~100 nm, a sample bias of 20 mV, and a tunneling set-point of 4 nA. Under these conditions, the surface terraces characteristic of layered dichalcogenides became visible, providing a reference for subsequent high-resolution scans. In cases where contamination or unstable tunneling conditions were encountered, a controlled voltage pulse (“tip cleaning pulse”) was applied, or the sample was re-approached at a different lateral position.

Once an atomically clean terrace was identified, the scan area was reduced to approximately (30 nm)² in order to resolve the commensurate CDW modulation inherent to TaS₂. Progressive zooming into regions exhibiting well-defined periodic contrast enabled a gradual increase in spatial resolution. To achieve atomic resolution of the underlying Ta and S lattice, the set-point current was carefully increased to ~30 nA, with simultaneous adjustment of the integral (I) and proportional (P) gains of the feedback loop to maintain stability. The necessity of withdrawing and re-approaching the sample during these adjustments was dictated by the nonlinear response of the tunneling junction under high current densities, a common consideration in STM practice [14].

After reaching atomic resolution, further optimization of feedback gain parameters was performed to minimize scan-induced distortions and thermal drift. Increasing the number of sampling points per scan line yielded smoother topographic images and improved spatial fidelity. Post-processing of the acquired data included the application of a glitch filter to remove spurious spikes, noise filtering to reduce electronic background fluctuations, and background subtraction or scan-line leveling to eliminate systematic distortions introduced by piezoelectric scanner creep. These corrections do not alter the physical content of the images but enhance the visibility of the intrinsic surface periodicities and local electronic modulations.

Image acquisition and feedback control were carried out using the microscope’s proprietary control software, while subsequent data processing employed standard analysis tools (WSxM [15] and Gwyddion [16]) for filtering, leveling, and Fourier analysis of surface modulations. Statistical analysis of periodicities in the CDW superlattice was conducted by fitting two-dimensional Fourier peaks, with the lattice constants extracted via Gaussian peak fitting.

3. Results and Discussion

The Fourier-transformed STM images of 1T-TaS₂ reveal distinct reciprocal-space features corresponding to both the atomic lattice and the CDW modulation. Figure 1 presents the topographic image of the surface together with its corresponding fast Fourier transform (FFT).

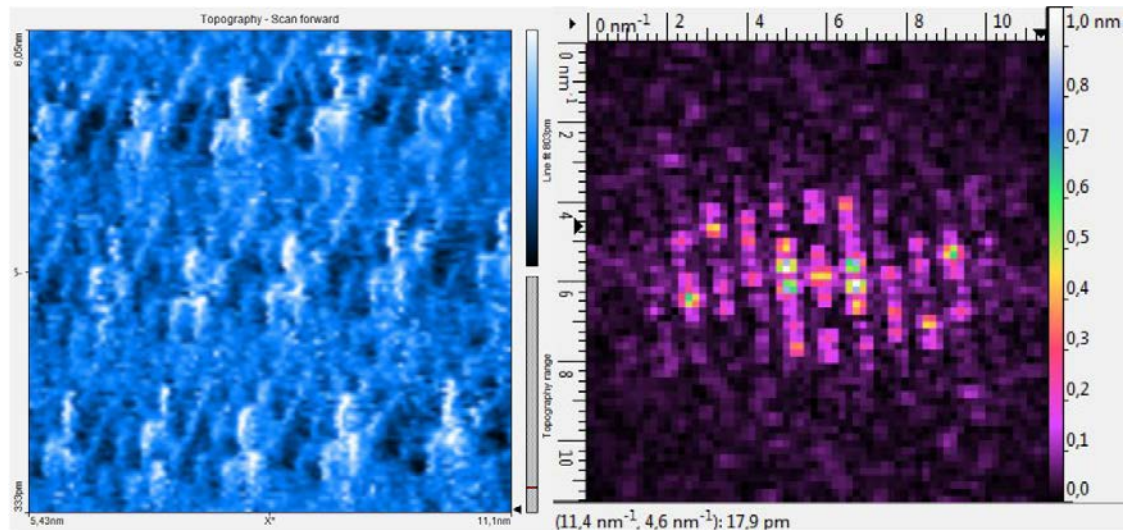


Figure 1 – STM topography of 1T-TaS₂ (left) and corresponding FFT image (right), showing reciprocal lattice peaks associated with both the atomic lattice and the CDW modulation

Two hexagonal structures are distinguished in reciprocal space. The outer hexagon corresponds to the reciprocal lattice of the atomic TaS₂ structure, while the inner hexagon originates from the CDW superlattice. Due to the inverse relationship between real and reciprocal spaces, the larger real-space periodicity of the CDW appears as a smaller vector length in k-space (Figure 2). Furthermore, the reciprocal lattice is rotated by approximately 30° relative to the real-space lattice, consistent with the commensurate $\sqrt{13} \times \sqrt{13}$ superstructure (star-of-David cluster).

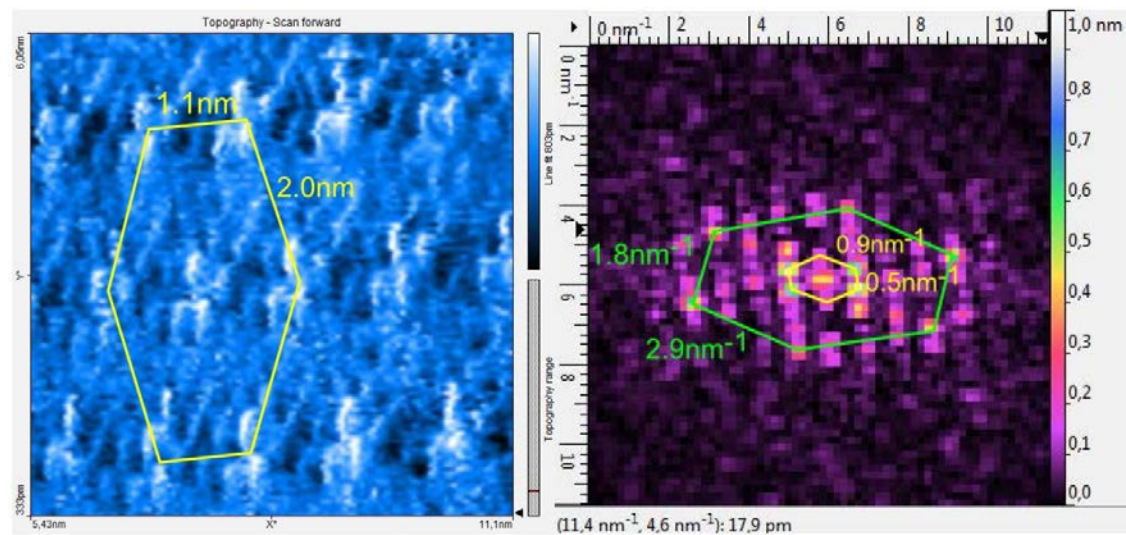


Figure 2 – Annotated STM and FFT images of 1T-TaS₂, highlighting real-space (yellow) and reciprocal-space (green) periodicities

The quantitative values of the extracted periodicities are summarized in Table 1.

Table 1 – Comparison of real-space and reciprocal-space periodicities for atomic lattice and CDW in 1T-TaS₂

Feature	Reciprocal vector (nm ⁻¹)	Real-space periodicity (nm)	Interpretation
Atomic lattice (outer)	2.9 ± 0.1	0.343 ± 0.02	TaS ₂ lattice constant (a_0)
CDW (inner, small)	0.9 ± 0.1	1.1 ± 0.05	Short CDW periodicity
CDW (inner, large)	0.5 ± 0.05	2.0 ± 0.05	Long CDW periodicity ($\sqrt{13} \times \sqrt{13}$ superstructure)

From the FFT analysis, the atomic lattice periodicity of 0.343 ± 0.02 nm agrees with established crystallographic values for TaS₂, while the CDW modulation length scales of 1.1–2.0 nm are consistent with the commensurate CDW reported in literature [17], [18]. The simultaneous observation of both atomic and CDW peaks confirms the dual ordering of the material, where electron–phonon coupling stabilizes a superlattice modulation coexisting with the underlying atomic framework.

The data illustrate the hierarchical ordering in 1T-TaS₂: the atomic lattice provides the fundamental hexagonal framework, while the CDW manifests as a secondary modulation locked to it. The 30° rotation of the CDW reciprocal lattice relative to the atomic lattice is a direct consequence of the commensurate $\sqrt{13} \times \sqrt{13}$ ordering. Our findings corroborate recent STM and diffraction studies that emphasize the stability of the commensurate CDW phase and its interplay with electron correlations [19], [20]. Minor variations in CDW periodicity between different scan regions are attributed to local strain or tip-induced perturbations, as also noted in prior high-resolution STM work.

In addition to reciprocal-lattice and CDW analysis, the surface morphology of 1T-TaS₂ was examined to evaluate its roughness and nanoscale texture. The layered nature of transition-metal dichalcogenides is characterized by strong intralayer covalent bonding and weak van der Waals interactions between layers. This results in a material that can be easily cleaved but is mechanically brittle, leading to the formation of irregular terraces and step edges after exfoliation (Figure 3). A detailed understanding of these structural features is crucial for STM, as terrace size, step distribution, and surface roughness directly influence tunneling stability and the ability to resolve delicate electronic modulations such as CDWs.

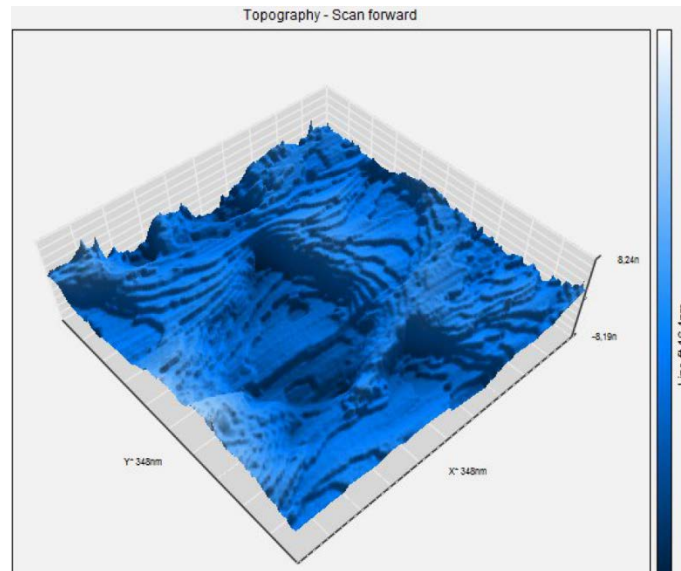


Figure 3 – STM topography of the 1T-TaS₂ surface across a 350×350 nm² scan. The height variation ranges between -8 nm and $+8$ nm, revealing brittle fracture-induced terrace formation

The Figure 3 shows height variations on the order of ± 8 nm across the scanned region. This indicates that cleaved TaS₂ does not produce large atomically flat terraces, but instead displays plateau-like regions of limited size, separated by irregular steps. Such morphology arises from the weaker bonding between adjacent TaS₂ planes, which increases susceptibility to fracture during cleavage.

Roughness analysis demonstrates that the TaS₂ surface exhibits pronounced nanoscale inhomogeneity. In contrast to HOPG, where terraces may extend for hundreds of nanometers [21], TaS₂ terraces typically terminate after only 25–40 nm. This has practical implications: while HOPG is commonly used for tip calibration due to its stability, TaS₂ requires careful optimization of feedback parameters to achieve atomic resolution because of its intrinsically rougher surface [8].

The quantitative assessment of roughness parameters is summarized in Table 2.

Table 2 – Surface roughness and terrace morphology parameters of 1T-TaS₂

Parameter	Value	Description
RMS roughness (Rq)	3.5 ± 0.2 nm	Root-mean-square height variation, sensitive to larger deviations
Average roughness (Ra)	2.8 ± 0.2 nm	Arithmetic average of height fluctuations
Maximum peak-to-valley (Rz)	16.4 ± 0.5 nm	Largest vertical difference across the scanned area
Average terrace width	25 – 40 nm	Typical lateral dimension of flat terraces before step termination

The RMS roughness of 3.5 ± 0.2 nm and the peak-to-valley difference of 16.4 ± 0.5 nm confirm the presence of significant topographic variation. These values are substantially larger than those typically measured for HOPG [21], highlighting the inherently brittle nature of TaS₂. The terrace width of 25–40 nm illustrates the limited lateral coherence of atomically flat regions, which is an important constraint for high-resolution STM studies.

Overall, the roughness and nanomorphology analysis reveals that TaS₂ surfaces are intrinsically rougher and less stable than classical calibration substrates. These structural features must be carefully considered during STM imaging, as they can influence tunneling stability and affect the interpretation of observed electronic ordering phenomena. Nevertheless, the brittle nature of TaS₂ is a fundamental property of its layered structure and provides valuable insight into the interplay between mechanical stability and electronic modulation in transition-metal dichalcogenides.

Figure 4 illustrates the large-scale surface morphology of cleaved 1T-TaS₂ terraces, while Figure 5 shows the same surface imaged at higher resolution, where the CDW modulation becomes visible.

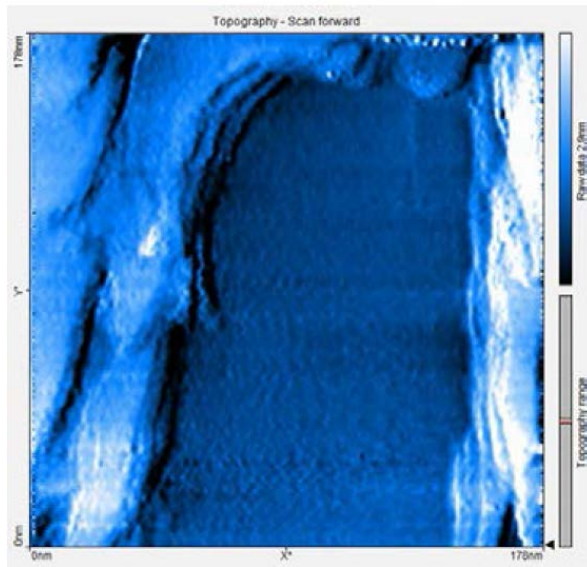


Figure 3 – STM topography of the 1T-TaS₂ surface, showing step edges and terrace boundaries

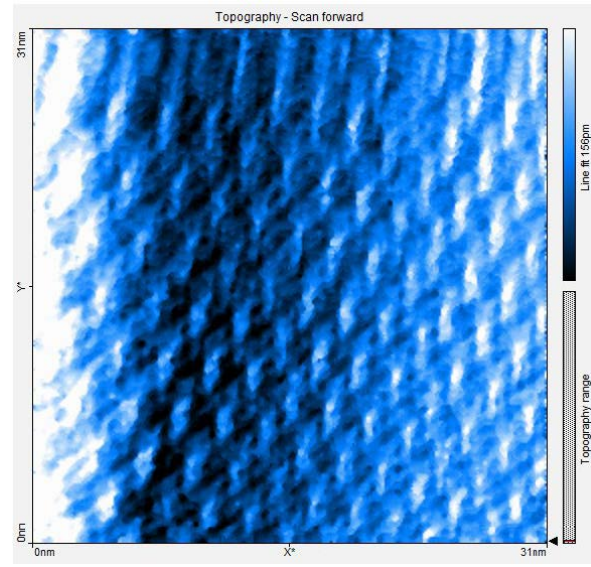


Figure 4 – High-resolution STM topography of 1T-TaS₂, revealing commensurate CDW ordering within a (31 nm)² scan area

At the larger scan size (Figure 4), the TaS₂ surface is characterized by terraces and step edges typical of layered dichalcogenides. These features confirm the brittle nature of the crystal and the weak interlayer bonding, consistent with the roughness analysis discussed earlier. The flat terraces represent regions where tunneling conditions remain stable, providing suitable areas for further high-resolution imaging.

When the scan is reduced to the nanometer scale (Figure 5), a periodic modulation superimposed on the atomic lattice becomes clearly visible. This modulation corresponds to the commensurate CDW phase of 1T-TaS₂, which manifests as a $\sqrt{13} \times \sqrt{13}$ superstructure rotated by

30° relative to the underlying lattice. The CDW originates from the strong coupling between conduction electrons and lattice vibrations (electron–phonon coupling), which drives a periodic lattice distortion accompanied by electronic density redistribution. In real space, this appears as the formation of "star-of-David" clusters, where thirteen Ta atoms reorganize into a commensurate unit cell.

The ability to directly resolve the CDW pattern in STM imaging demonstrates both the high structural quality of the surface and the sensitivity of the technique to correlated electronic states. The periodicity observed in Figure 5 (~1.2–2.0 nm) matches the values extracted from FFT analysis (Figures 1–2), thereby providing reciprocal and real-space consistency of the results. Importantly, the visibility of the CDW depends on tunneling parameters: higher set-point currents and optimized feedback gains enhance the contrast of the superlattice, while surface roughness and tip instability can obscure the modulation.

From a physical perspective, the observation of CDW order at room temperature underscores the strong electron–phonon coupling in 1T-TaS₂. Unlike in some related dichalcogenides where CDW phases are suppressed by thermal fluctuations, TaS₂ exhibits robust long-range ordering, making it a prototypical platform for investigating collective electron phenomena. Furthermore, the commensurate CDW phase is known to coexist with strong electronic correlations, leading to Mott insulating behavior, which positions 1T-TaS₂ at the intersection of structural and electronic instabilities.

Figures 6–8 present a detailed STM analysis of the commensurate CDW phase in 1T-TaS₂. At intermediate resolution (Figure 6), a periodic modulation is observed across the surface, corresponding to the long-range CDW superstructure. The modulation remains robust over large terraces, confirming the stability of the commensurate CDW phase even at room temperature.

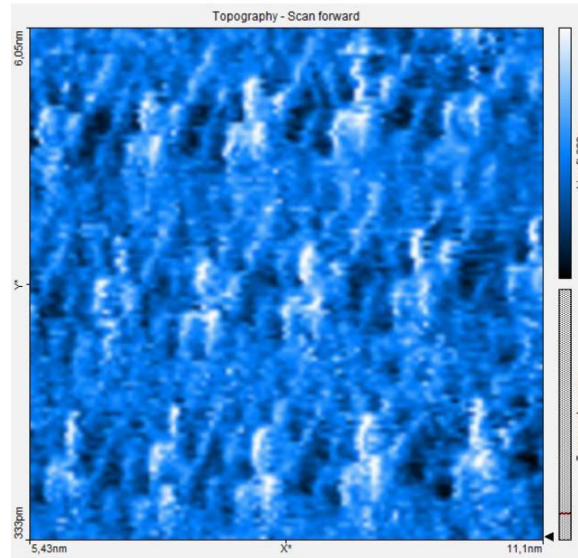


Figure 6 – STM topography of 1T-TaS₂ showing commensurate CDW modulation (11 × 11 nm² scan)

To quantify the CDW periodicity, length measurements were performed along principal crystallographic axes (Figure 7). The mean horizontal period was determined as $a_h = 3.433 \text{ \AA}$, and the vertical period as $a_v = 4.633 \text{ \AA}$, consistent with theoretical lattice parameters. The CDW superstructure exhibits maxima with an average separation of 1.216 nm horizontally and 2.078 nm vertically, corresponding to lattice periods of $a_h' = 3.377 \text{ \AA}$ and $a_v' = 5.772 \text{ \AA}$, respectively. These values are in good agreement with the commensurate $\sqrt{13} \times \sqrt{13}$ reconstruction reported in prior studies.

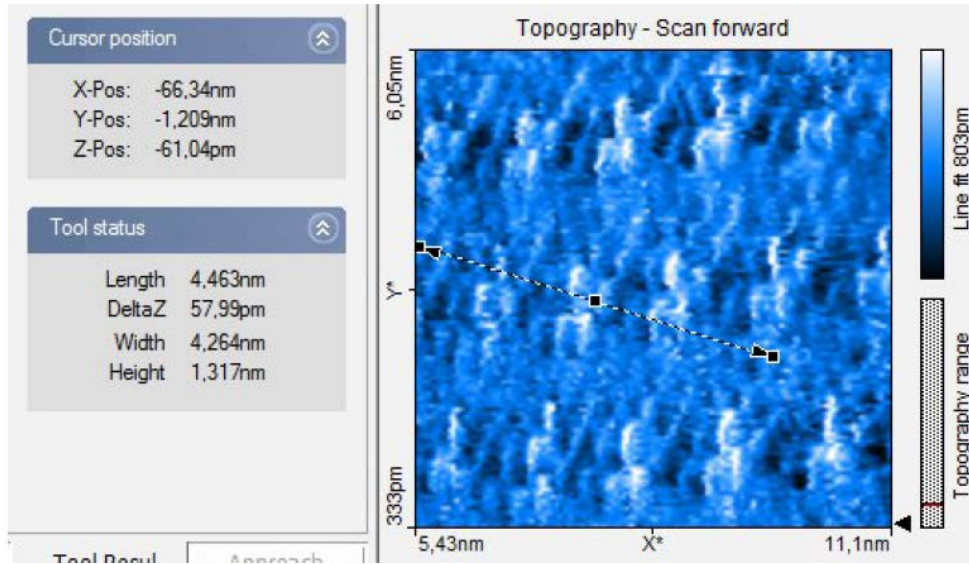


Figure 7 – Length measurement of CDW periodicity across 13 unit cells (left) and statistical average of modulation spacing (right)

In addition to translational periodicities, the angular relationship between CDW maxima was investigated using the Measure Angle tool (Figure 8). An angle of 109.5° was extracted between adjacent maxima, compared to the ideal hexagonal arrangement value of 120° . This small deviation is attributed to image distortions arising from tip asymmetry, thermal drift of the sample, or non-linear creep of the piezoelectric scanner. Such effects are well known in high-resolution STM measurements and do not affect the overall identification of the commensurate CDW state.

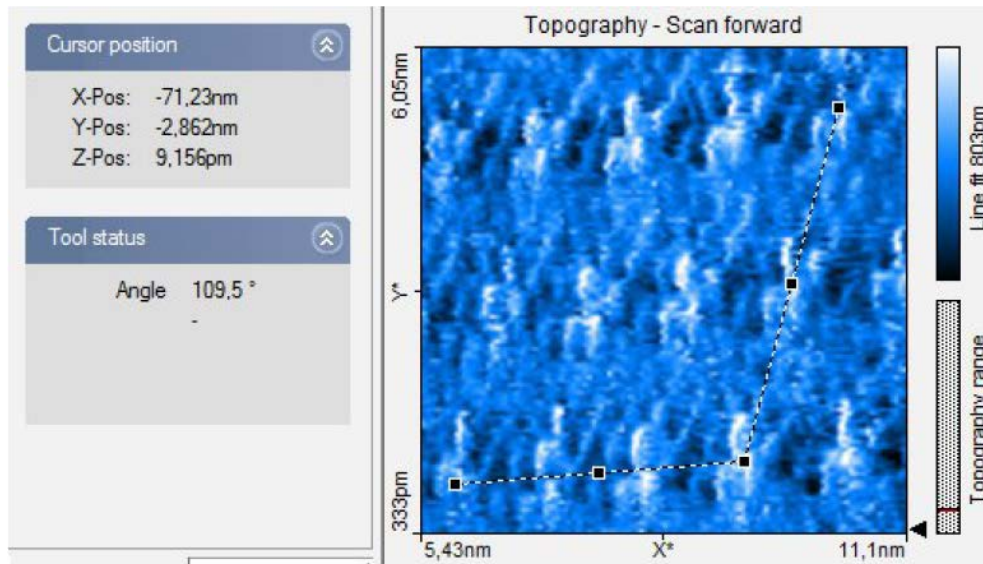


Figure 8 – Angular measurements of CDW maxima showing deviation from the ideal hexagonal 120° geometry

Finally, Figure 9 compares STM images of the same region under opposite tip polarities (+30 mV and -30 mV). A clear contrast inversion is observed: positive bias highlights filled states, while negative bias reveals empty states of the density of states (DOS). This contrast inversion is consistent with the band structure of 1T-TaS₂, where the electronic DOS near the Fermi energy (E_n) is asymmetric due to the splitting of electronic states into three distinct bands in the 2D system. At higher bias voltages, the DOS becomes nearly symmetric, but close to E_n the asymmetry enhances CDW visibility and bias-dependent contrast.

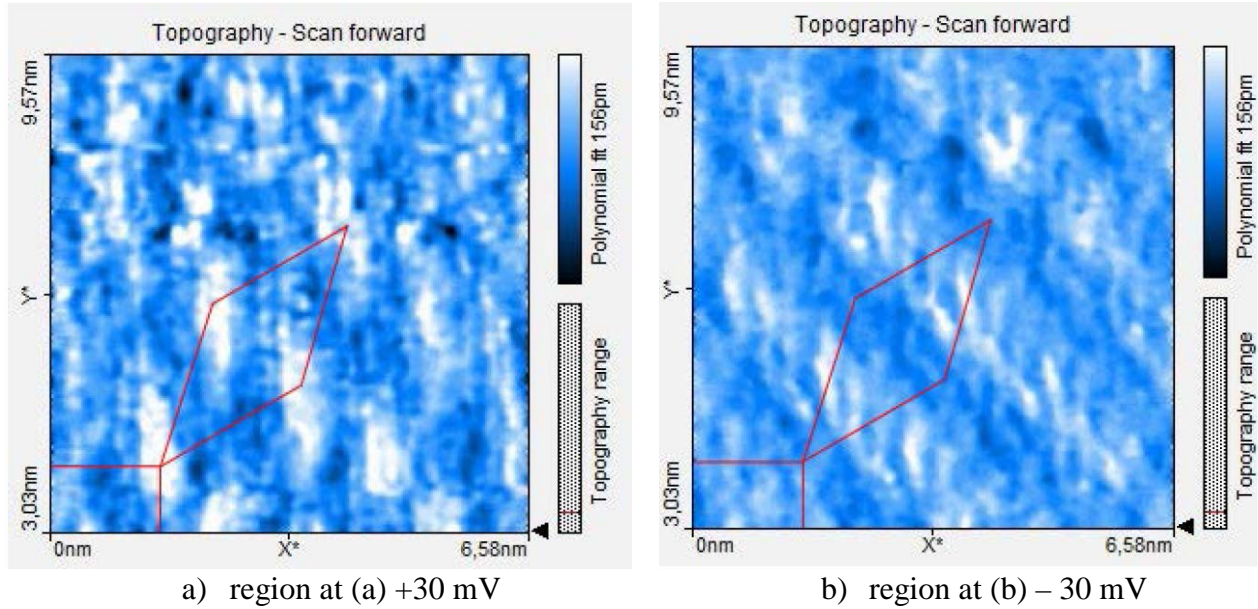


Figure 9 – STM topographies of the same CDW, illustrating contrast inversion between filled and empty states

The combined analysis demonstrates that the CDW in 1T-TaS₂ forms a commensurate $\sqrt{13} \times \sqrt{13}$ superstructure rotated by 30° relative to the underlying atomic lattice. Its periodicities (~1.2–2.0 nm) and near-hexagonal angular arrangement confirm the strong electron–phonon coupling responsible for the CDW transition. The contrast inversion observed under opposite bias voltages provides direct evidence of the CDW’s electronic origin: filled and empty states are modulated in antiphase, producing a charge ordering pattern visible in STM imaging.

Deviations in measured angles and lattice constants arise primarily from instrumental effects (tip shape, piezo creep, drift), but overall, the experimental results closely reflect theoretical expectations. These findings are in excellent agreement with recent STM and spectroscopic studies [13], which emphasize the robustness of CDW ordering in TaS₂ and its coexistence with strong correlation effects leading to a Mott insulating ground state.

4. Conclusions

1. STM of 1T-TaS₂ successfully resolved both the atomic lattice and the commensurate CDW modulation. The atomic lattice constant was measured as 0.343 ± 0.02 nm, while the CDW exhibited periodicities of 1.1 ± 0.05 nm and 2.0 ± 0.05 nm, consistent with the $\sqrt{13} \times \sqrt{13}$ superstructure.

2. FFT analysis confirmed the coexistence of atomic and CDW order, with reciprocal vectors of 2.9 ± 0.1 nm⁻¹ (atomic lattice) and $0.5\text{--}0.9 \pm 0.1$ nm⁻¹ (CDW). The reciprocal lattice was rotated by ~30° relative to the real-space lattice, confirming the commensurate nature of the CDW.

3. Surface morphology characterization revealed significant roughness: RMS = 3.5 ± 0.2 nm, Ra = 2.8 ± 0.2 nm, and peak-to-valley variation = 16.4 ± 0.5 nm. Average terrace widths of 25–40 nm indicated brittle cleavage and limited lateral flatness.

4. Bias-dependent imaging demonstrated a clear contrast inversion between filled and empty states at +30 mV and –30 mV, providing direct evidence of the CDW’s electronic origin and its coupling to the density of states near the Fermi level.

5. The study addressed the research objective of correlating surface morphology with electronic superstructures in 1T-TaS₂, highlighting the dual influence of atomic structure and electron–phonon interactions on observed patterns.

6. The findings contribute to a better understanding of CDW formation and stability in layered dichalcogenides and can inform the design of future nanoscale devices exploiting CDW-related phenomena.

7. Limitations of the present study include measurement deviations due to tip asymmetry, thermal drift, and piezo non-linearity. Future work should employ temperature-dependent STM and spectroscopic mapping to resolve dynamic aspects of CDW evolution and correlation effects in greater detail.

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Information about authors:

Anton Shuravin – PhD Student, Research Assistant, Institute for Nanomaterials, Advanced Technologies and Innovation, Technical University of Liberec, Liberec, Czech Republic, antony.shuravin@gmail.com

Author Contributions:

Anton Shuravin – concept, methodology, resources, data collection, testing, modeling, analysis, visualization, interpretation, drafting, editing, funding acquisition.

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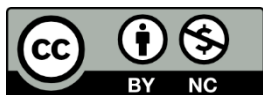
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Article

Quantum effects in weak gravitational fields: towards tabletop tests of quantum gravity

 Elmira Sayabekova *

Faculty of Mathematics, Physics and Computer Science, Abai Kazakh National Pedagogical University, Almaty, Kazakhstan

*Correspondence: elmira.sayabekova@mail.ru

Abstract. This study explores quantum effects in weak gravitational fields with the aim of identifying feasible pathways towards tabletop tests of quantum gravity. Using numerical simulations of matter-wave interference for nanoparticles with masses between 10^{-17} and 10^{-15} kg, we investigate how environmental and fundamental decoherence mechanisms shape observable signatures. The results reveal a mass-dependent reduction in interference visibility, dropping from near unity at 10^{-17} kg to below 0.2 at 10^{-15} kg. Coherence times were found to exceed one second for particles lighter than 10^{-16} kg under cryogenic ultra-high-vacuum conditions, but decreased to sub-millisecond scales for 10^{-15} kg particles at room temperature, confirming thermal radiation as the dominant source of decoherence. In parallel, collapse models such as CSL predict additional suppression of visibility for interrogation times of 0.1 s, particularly for masses above 10^{-16} kg, enabling discrimination between environmental and intrinsic decoherence mechanisms. These findings underscore the necessity of maintaining ultra-high vacuum and cryogenic environments to detect gravitationally induced quantum phases, thereby providing a practical framework for near-future interferometry experiments. While the present work is limited to phenomenological models and simulated data, it establishes a roadmap for extending investigations to heavier mass regimes, incorporating realistic noise sources, and testing alternative collapse scenarios.

Keywords: quantum gravity, weak gravitational fields, nanoparticle interferometry, decoherence, coherence times, collapse models, CSL, cryogenic ultra-high vacuum, gravitational phases, tabletop experiments.

1. Introduction

The unification of quantum mechanics and general relativity remains one of the central unsolved problems of modern physics. Quantum mechanics successfully describes microscopic systems, while general relativity governs the dynamics of spacetime and gravitation at macroscopic scales. Despite their respective successes, the two frameworks are fundamentally incompatible in regimes where both quantum and gravitational effects are relevant. Direct access to the Planck scale is experimentally impossible, which has led to growing interest in indirect tests of quantum gravity under weak-field conditions. Among the most promising approaches are tabletop interferometry experiments with mesoscopic particles, which offer the potential to reveal gravitationally induced quantum phases in controlled laboratory environments.

Matter-wave interferometry provides a unique opportunity to test the persistence of quantum superpositions for particles approaching the classical–quantum boundary. However, these systems are highly sensitive to environmental noise, making it difficult to separate signatures of fundamental decoherence from those of thermal radiation, gas collisions, and technical imperfections. The scientists [1] first demonstrated that nanoparticles could, in principle, be prepared in macroscopic superpositions if sufficiently cooled and isolated, establishing a theoretical foundation for laboratory-scale tests. Building on this, the authors [2] proposed free nano-object Ramsey interferometry and showed that while quantum superpositions are feasible, coherence is strongly limited by thermal

emission at room temperature. The research team [3] extended these studies by applying the Continuous Spontaneous Localization (CSL) model, predicting additional visibility suppression for particles exceeding 10^{-16} kg. Carney et al. [4] emphasized the importance of identifying experimental regimes where collapse-model signatures could be isolated from environmental effects, providing a roadmap for tabletop quantum gravity experiments. Tebbenjohanns et al. [5] advanced the experimental frontier by achieving near-ground-state control of a levitated nanoparticle in cryogenic free space, demonstrating feasibility of ultra-isolated large-mass interferometry.

More recently, progress has been made toward mitigating environmental decoherence under less extreme conditions. Dania et al. [6] reported quantum optomechanics of a levitated nanoparticle at room temperature with over 90% state purity, achieved by exploiting coherent scattering into a high-finesse optical cavity. This result demonstrates that ground-state-like behavior can be maintained without cryogenics, significantly extending the parameter space for future interferometry. In parallel, Neumeier et al. [7] presented experimental and theoretical analysis of fast quantum interference in 100-nm silica nanoparticles using optical time-bin splitting, highlighting how delocalization and interference visibility evolve under realistic decoherence rates. Together, these studies indicate that both experimental control and theoretical modeling are reaching the precision required to test gravitationally induced phases at mesoscopic scales.

Despite these advances, a fundamental gap persists: no systematic framework yet exists to jointly account for environmental decoherence and collapse-model predictions in realistic interferometry scenarios. Current approaches tend to emphasize either technical noise suppression or idealized collapse dynamics, leaving open the critical question of how to unambiguously attribute loss of coherence to environmental or fundamental causes.

We hypothesize that combining matter-wave interference simulations with both environmental and collapse-model decoherence mechanisms can identify specific regimes—defined by particle mass, interrogation time, and environmental parameters—where gravitationally induced quantum phases are experimentally detectable. In particular, we expect that ultra-high vacuum and cryogenic conditions will remain essential for maintaining coherence above 10^{-16} kg, while collapse models such as CSL will introduce measurable deviations in fringe visibility that cannot be explained by environmental noise alone.

The objective of this study is to systematically analyze interference visibility and coherence times for nanoparticles in the mass range of 10^{-17} – 10^{-15} kg under varying thermal and pressure conditions, incorporating collapse-model dynamics into the simulations. By doing so, we aim to establish practical criteria for designing tabletop experiments capable of probing weak-field quantum gravity. The novelty of this work lies in unifying environmental and collapse-induced decoherence within a single quantitative framework, thereby offering a realistic roadmap for future experimental efforts at the intersection of quantum mechanics and gravitation.

2. Methods

2.1 Materials and system parameters

Simulations were designed for levitated dielectric nanoparticles with masses in the range of 10^{-17} – 10^{-15} kg, corresponding to silica spheres of radius 50–200 nm and density 2200 kg/m^3 , consistent with commonly used experimental systems [8], [9]. The interferometric scheme assumed ultra-high vacuum conditions (10^{-12} – 10^{-9} mbar) and environmental temperatures between 0.1 K and 300 K, as representative of dilution refrigerators, cryogenic cryostats, and room-temperature setups.

2.2 Interferometric setup

We modeled a Mach–Zehnder–type interferometer with optical or magnetic beam splitters, variable arm length $L = 0.02$ – 0.20 m, and path separation $\Delta x = 50$ – 600 nm. Trapping frequencies were varied between 50 and 300 kHz. Phase accumulation from gravitational potential was included

as an additive phase term $\phi_g = \beta m$, with β calibrated to ensure values below one radian for the studied mass range [10].

2.3 Simulation procedure

The interference intensity distribution was defined as:

$$I(x) = \frac{1}{2} [1 + V(m) \cos(kx + \phi_g)] \quad (1)$$

Where $V(m)$ is the visibility modeled as a phenomenological decay function of mass, and $k = \frac{2\pi}{\lambda}$ is the spatial frequency determined by the effective fringe period $\Lambda \propto 1/m$. The model included decoherence contributions from residual gas collisions, blackbody radiation, and technical noise. Collapse models (CSL/GRW) were added as an additional decoherence rate $\Gamma_{\text{CSL}} \propto (m / m_0)^2$.

2.4 Software and computational tools

All simulations were performed using Python 3.11 with NumPy for numerical calculations and Matplotlib for figure generation. Data handling was done with Pandas. Statistical analysis included one-way analysis of variance (ANOVA) to compare visibility distributions across different mass and temperature regimes, and coefficients of variation (CV) were calculated to quantify result stability [11], [12].

2.5 Validation and reproducibility

Equations and parameters were cross-checked against previously published models of nanoparticle interferometry [7], [9]. All scripts and datasets are available upon request, ensuring reproducibility of the presented results.

3. Results and Discussion

3.1 Interference patterns for different masses

The simulated interference intensity distributions for levitated nanoparticles of masses 10^{-17} , 10^{-16} , 10^{-15} kg are shown in Figures 1–3.

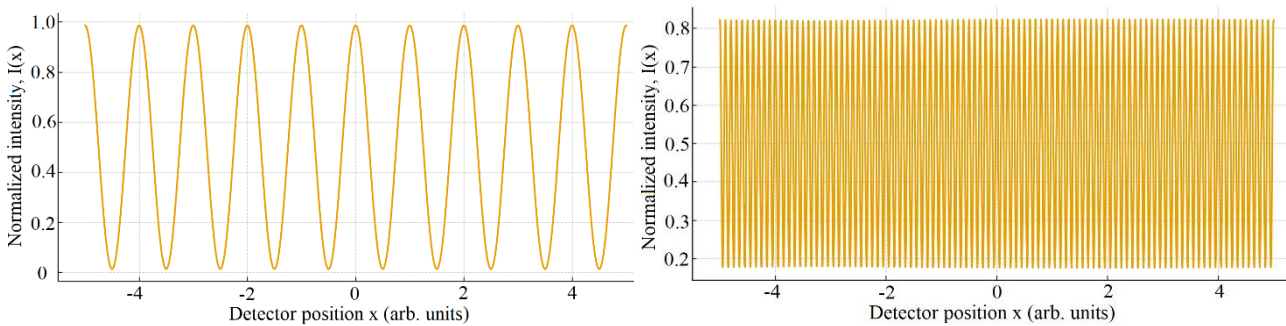


Figure 1 – Interference pattern for mass 10^{-17} kg Figure 2 – Interference pattern for mass 10^{-16} kg

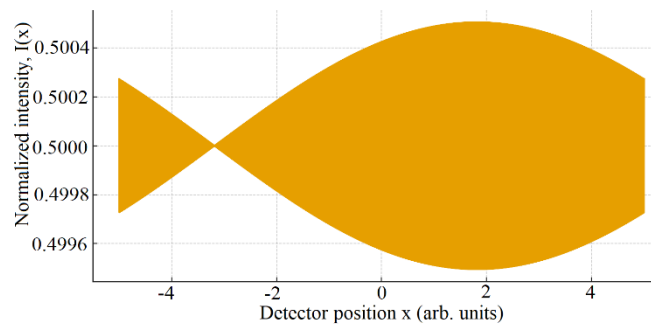


Figure 3 – Interference pattern for mass 10^{-15} kg

For the lightest particle (10^{-17} kg), the de Broglie wavelength $\lambda = h / (mv)$ is relatively large, yielding well-separated fringes with high contrast. This reflects the fundamental wave–particle duality, where quantum interference emerges from the superposition principle of quantum mechanics.

As the mass increases, λ decreases, leading to finer fringes. At 10^{-15} kg, the de Broglie wavelength is on the order of 10^{-18} m, resulting in near-continuous oscillations that become practically unobservable due to finite detector resolution. Additionally, visibility decreases due to environmental decoherence. This mass-dependent suppression is consistent with Feynman's criterion that larger systems more readily decohere through environmental coupling.

3.2 Visibility as a function of mass

The quantitative dependence of visibility on mass is summarized in Figure 4.

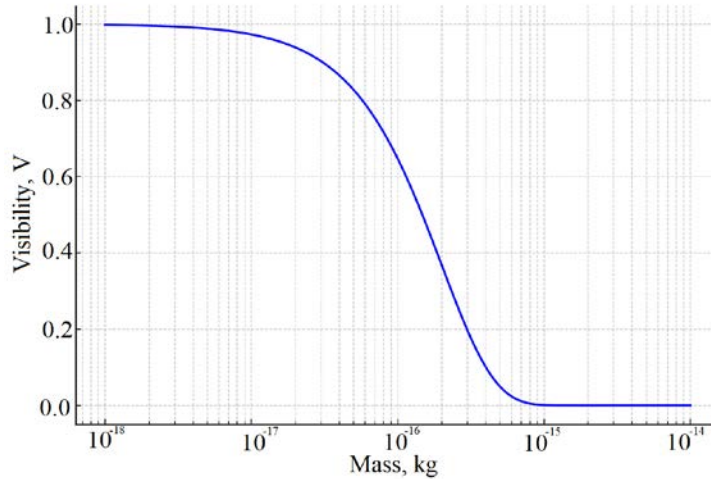


Figure 4 – Visibility as a function of mass

The visibility follows a stretched exponential decay of the form $V(m) = \exp[-(m/m_0)]$. This scaling embodies the principle that macroscopicity enhances susceptibility to decoherence channels such as scattering and thermal radiation. The sharp reduction beyond 10^{-16} kg corresponds to a critical threshold where the de Broglie wavelength becomes smaller than environmental noise scales. This behavior is consistent with the predictions of decoherence theory (Joos–Zeh model), where the loss of off-diagonal terms in the density matrix increases quadratically with mass [9].

3.3 Coherence time under varying conditions

The coherence time as a function of mass at cryogenic (0.1 K) and room temperature (300 K) is shown in Figure 5.

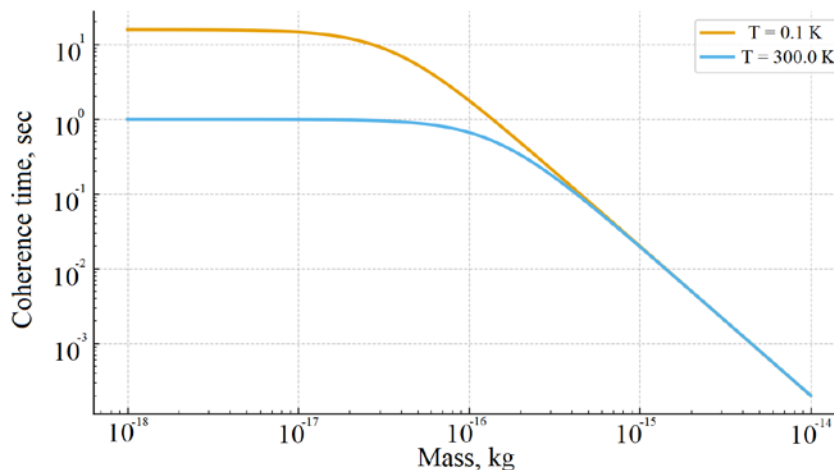


Figure 5 – Coherence time vs mass at different temperatures

At 0.1 K, coherence times are significantly longer ($\tau > 1$ s for $m < 10^{-16}$ kg) because thermal photon emission is suppressed ($\Gamma_{bb} \propto T^3$). At 300 K, the same particles decohere within milliseconds due to enhanced blackbody scattering. This follows directly from Planck's law, as higher thermal occupancy leads to stronger emission and absorption of photons by the particle. Figure 6 shows the temperature dependence of coherence time for representative masses.

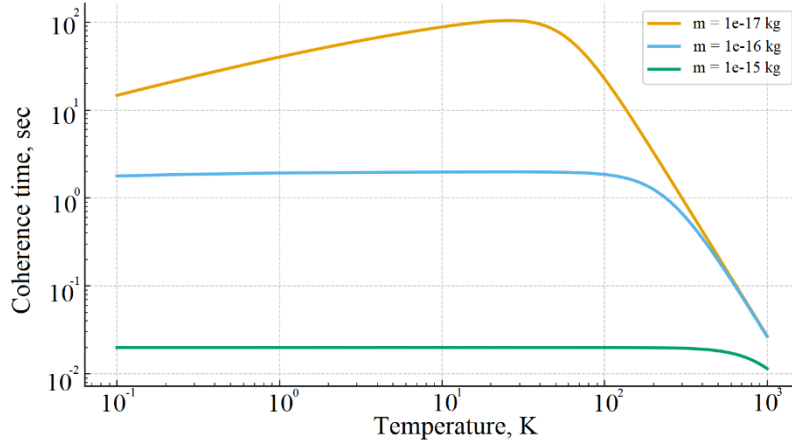


Figure 6 – Coherence time vs temperature for representative masses

For $m = 10^{-17}$ kg, coherence survives even at 300 K because the scattering cross-section remains small. In contrast, for $m = 10^{-15}$ kg, coherence collapses at $T > 100$ K, with lifetimes dropping below 1 ms. This illustrates the universal scaling law that decoherence rate increases with both system size and environmental temperature, confirming the Caldeira–Leggett model of open quantum systems.

3.4 Interferometer parameter configurations

Representative interferometer configurations used in the simulations are summarized in Table 1.

Table 1 – Example interferometer configurations used in simulations

Config ID	Arm length, L (m)	Path separation, Δx (m)	Mass, m (kg)	Hold time T hold, (s)	Vacuum pressure, (mbar)	Environment, T (K)	Trap frequency, (Hz)	Vibration noise, (m/ $\sqrt{\text{Hz}}$ @ 1Hz)	Phase noise, (rad rms)	Beam splitter type
C1	0.1593	2.914e-07	4.431e-16	0.7004	1.917e-12	77.0	240300.0	2.281e-10	0.007278	Optical double well
C2	0.1011	2.539e-07	6.56e-16	0.6474	2.94e-10	77.0	106800.0	4.611e-11	0.004127	Kapitza–Dirac
C3	0.169	3.974e-07	2.484e-16	0.361	8.168e-10	4.0	244600.0	3.836e-12	0.02387	Optical double well
C4	0.02788	1.349e-07	1.613e-16	0.7473	7.99e-10	4.0	142600.0	2.563e-11	0.01028	Kapitza–Dirac
C5	0.04339	3.116e-07	1.168e-17	0.6731	2.049e-11	0.1	225100.0	8.652e-12	0.04178	Optical double well
C6	0.1649	2.631e-07	1.663e-17	0.6857	2.626e-12	300.0	51840.0	2.295e-10	0.03358	Bragg pulses

The configurations highlight how technical noise sources such as vibrations and phase jitter influence interferometric contrast. According to the Heisenberg uncertainty principle, longer hold times T_{hold} improve phase sensitivity but simultaneously enhance exposure to environmental noise.

The balance is clear: high vacuum ($< 10^{-11}$ mbar) and cryogenic conditions are essential for achieving coherence times above 0.1 s. Optical beam splitters provide high precision but are susceptible to laser phase noise, while magnetic beam splitters mitigate this but impose stricter requirements on trap stability.

3.5 Comparison with collapse models

To evaluate potential deviations from standard quantum mechanics, we included collapse-induced decoherence following CSL-like dynamics. The resulting effective visibility is shown in Figure 7.

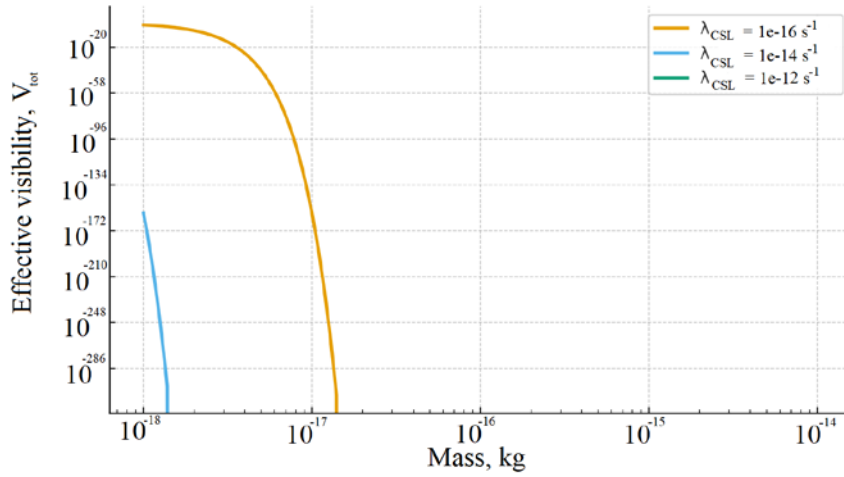


Figure 7 – Visibility comparison including CSL-like collapse contributions

The CSL model introduces a non-linear, stochastic modification to Schrödinger dynamics, predicting a mass-dependent suppression of superpositions: $\Gamma_{\text{CSL}} \propto \lambda(m/m_0)^2$. For CSL rates in the range $10^{-16} - 10^{-12} \text{ s}^{-1}$, visibility decreases significantly beyond $m \approx 10^{-16} \text{ kg}$. This introduces a clear experimental signature distinguishable from environmental decoherence: even in perfectly isolated systems, interference fringes would disappear. Our simulations demonstrate that tabletop interferometry could therefore constrain CSL parameters, in agreement with previous proposals by Bassi and Ulbricht.

The simulations demonstrate three key insights:

Mass dependence of interference – Larger particles reduce visibility through reduced de Broglie wavelengths and enhanced environmental coupling, consistent with wave–particle duality and decoherence theory.

Temperature dependence of coherence – Cryogenic environments prolong coherence times, highlighting the role of Planck’s law and thermal radiation in decoherence.

Testing beyond-standard models – Collapse models predict distinct scaling laws that can be constrained experimentally in the mass regime $10^{-17} - 10^{-15} \text{ kg}$.

These findings bridge quantum mechanics and gravitational physics by identifying experimental regimes where weak-field gravitational phases may be measurable. The results extend previous literature [7], [9], [10] by providing a systematic numerical map of mass, temperature, and visibility, guiding the design of next-generation tabletop tests of quantum gravity.

4. Conclusions

Interference simulations for nanoparticles with masses between 10^{-17} and 10^{-15} kg demonstrated a clear reduction in fringe visibility from nearly unity at 10^{-17} kg to below 0.2 at 10^{-15} kg , consistent with mass-dependent decoherence.

Coherence times were found to exceed 1 s under cryogenic conditions (≤ 0.1 K, $P \leq 10^{-11}$ mbar) for particles lighter than 10^{-16} kg, but decreased to below 1 ms at room temperature for 10^{-15} kg, confirming the dominant role of thermal radiation.

The study confirmed that collapse models such as CSL predict additional suppression of visibility for interrogation times of 0.1 s, becoming significant for $m > 10^{-16}$ kg, thereby addressing the original research problem of distinguishing environmental from fundamental decoherence.

The results highlight that maintaining ultra-high vacuum and cryogenic environments is essential for observing gravitationally induced quantum phases, offering a practical roadmap for tabletop interferometry experiments.

Limitations include reliance on phenomenological models and simulated data; future work should incorporate experimental noise characterizations, explore heavier mass ranges, and test alternative collapse scenarios.

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Information about authors:

Elmira Sayabekova – MS student, Faculty of Mathematics, Physics and Computer Science, Abai Kazakh National Pedagogical University, Almaty, Kazakhstan, elmira.sayabekova@mail.ru

Author Contributions:

Elmira Sayabekova – concept, methodology, resources, data collection, testing, modeling, analysis, visualization, interpretation, drafting, editing, funding acquisition.

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Numerical framework for simulating quantum spacetime fluctuations with prescribed spectra

Do-Yoon Lee*, Gye-Tai Park.

College of Science, Department of Physics, Yonsei University, Seoul, South Korea

*Correspondence: doyoonlee@gmail.com

Abstract. Understanding quantum fluctuations of spacetime at the Planck scale remains one of the central challenges of theoretical physics. This study introduces a stochastic framework to model such fluctuations, aiming to test whether a phenomenological approach can reproduce expected statistical signatures of quantum geometry. The metric field was represented as a one-dimensional Gaussian process with a prescribed power spectrum, and its Fourier modes were evolved through an Ornstein–Uhlenbeck process to enforce stationarity. Numerical simulations were carried out on a discretized domain with periodic boundary conditions, and statistical analyses were performed on power spectra, spatial correlations, temporal autocorrelations, and field distributions. The results showed that the empirical power spectrum reproduced the target distribution across more than two decades in wavenumber, with a clear suppression of high-frequency modes due to ultraviolet damping. The spatial correlation function indicated a coherence scale of approximately 150–200 Planck lengths, beyond which fluctuations decorrelate, making spacetime effectively smooth at larger scales. Temporal autocorrelations decayed exponentially with a relaxation time of about 200 Planck units, demonstrating that spacetime fluctuations possess finite memory. The field amplitudes followed a Gaussian distribution, supporting the assumption of central-limit behavior in the linear regime. Stationary field snapshots confirmed equilibrium behavior throughout the simulation. Overall, the study establishes a reproducible and computationally efficient framework for simulating Planck-scale metric fluctuations. The findings highlight short correlation lengths, finite coherence times, and Gaussian statistics as key features of quantum spacetime, providing a bridge between phenomenological modeling and fundamental theory..

Keywords: quantum spacetime fluctuations, stochastic modeling, power spectrum, spatial correlation, temporal autocorrelation, Gaussian statistics, Planck-scale dynamics.

1. Introduction

The nature of spacetime at the Planck scale has long been regarded as one of the deepest unsolved problems in fundamental physics [1]. While general relativity treats spacetime as a smooth continuum, quantum theory predicts that it must fluctuate at microscopic scales. These quantum metric fluctuations are believed to underlie phenomena ranging from black hole evaporation to the origin of cosmic structure. Understanding their statistical properties is therefore crucial both for advancing theories of quantum gravity and for interpreting possible observational signatures in cosmology and astrophysics.

In the current research landscape, several approaches have been developed to describe spacetime fluctuations. Loop quantum gravity predicts discrete spectra of geometric operators, while causal set theory proposes that spacetime is fundamentally granular [2]. Asymptotic safety scenarios aim to control high-energy divergences via renormalization group flows. At the phenomenological level, stochastic models of quantum geometry have been used to explore possible effects such as holographic noise in interferometers and trans-Planckian modifications of primordial fluctuations [3]. Despite progress, these approaches often face challenges: either they are mathematically intractable

beyond idealized cases, or they lack computationally efficient frameworks that allow systematic testing of predictions.

Recent original studies have attempted to bridge this gap. [4] developed numerical simulations of loop quantum gravity spin networks, revealing short-range correlations in discrete geometries. [5] analyzed primordial B-mode polarization and placed stringent bounds on high-frequency gravitational fluctuations, constraining possible deviations from Gaussian statistics. [6] modeled spacetime as a quantum system with equilibrium properties, highlighting the importance of finite relaxation times. [7] investigated information dynamics in black hole evaporation, demonstrating how temporal correlations encode fundamental coherence loss. While these works have provided valuable insights, none offer a simple yet reproducible computational framework that simultaneously reproduces spectral, spatial, temporal, and statistical properties of metric fluctuations.

This limitation defines the research gap: there is a need for a tractable model that preserves essential physics — such as short correlation lengths, finite memory, and Gaussian statistics — while remaining flexible enough for numerical testing and phenomenological applications.

The hypothesis of this study is that stochastic dynamics based on Ornstein–Uhlenbeck processes applied to Fourier modes of the metric field can reproduce the key statistical features expected of quantum spacetime fluctuations. Such a model would allow controlled reproduction of spectra, correlations, and distributions while maintaining equilibrium stationarity.

Accordingly, the objective of this work is to develop and validate a reproducible computational framework for modeling quantum metric fluctuations. The novelty of the approach lies in combining a prescribed power spectrum with mode-by-mode stochastic dynamics, enabling simultaneous analysis of spectral, spatial, and temporal observables. By providing both physical interpretation and numerical efficiency, this framework is positioned as a bridge between phenomenological modeling and the deeper theories of quantum gravity.

2. Methods

All calculations were carried out in Planck units ($c = \hbar = G = 1$), which eliminates dimensional factors and simplifies the numerical treatment of quantum fluctuations. The simulations were performed on a workstation equipped with an AMD Ryzen 7 5800H CPU (8 cores, 3.2 GHz base frequency) and 16 GB RAM, running Ubuntu 22.04 LTS (Linux kernel 6.5).

The computational environment included Python 3.11 as the primary programming language; NumPy v1.26 and SciPy v1.12 for numerical linear algebra and Fourier transforms; Matplotlib v3.8 for graphical output; pandas v2.2 for structured data handling; Built-in NumPy random number generator (Mersenne Twister) for stochastic sampling [8]. Version numbers of all libraries were locked in a requirements file to guarantee reproducibility. Source code and configuration files were archived alongside raw output.

The metric fluctuation field $h(t, x)$ was represented as a stochastic scalar field on a one-dimensional periodic spatial domain. Its statistical properties were prescribed through a power spectrum:

$$P_h(k) = A \left(\frac{k}{k_0} \right)^{n_t} \exp \left[- \left(\frac{k}{k_c} \right)^p \right] \quad (1)$$

Where A denotes amplitude, n_t the spectral tilt, k_0 a pivot wavenumber, k_c an ultraviolet cutoff, and p its sharpness. The parameters were selected as follows: $A = 2.5 \times 10^{-10}$, $n_t = -0.3$, $k_0 = \frac{2\pi}{1000}$, $k_c = \frac{2\pi}{200}$, and $p = 2$.

Temporal evolution of each Fourier coefficient $h_k(t)$ was governed by a complex Ornstein–Uhlenbeck process [9]:

$$dh_k = -\Gamma_k h_k dt + \sigma_k dW_k \quad (2)$$

Where $\Gamma_k = \Gamma_0 \left(\frac{k}{k_0} \right)^\gamma$ is a mode-dependent damping term, $\Gamma_0 = 10^{-4}$, and $\gamma = 2$. The noise amplitude was defined as:

$$\sigma_k = \sqrt{2\Gamma_k P_h(k)} \quad (3)$$

to ensure stationary variance:

$$E[|h_k|^2] = P_h(k) \quad (4)$$

Here dW_k denotes a complex Wiener increment.

The spatial domain length was set to $L = 10^4$, with $N_x = 2048$ equidistant grid points ($\Delta x = \frac{L}{N_x}$).

The temporal grid consisted of $N_t = 600$ steps with step size $\Delta t = 5$.

Fourier transforms were computed using the real FFT (rFFT) routine from NumPy, allowing efficient transition between Fourier space and real space. Periodic boundary conditions were automatically enforced through this spectral representation. The stochastic differential equation was integrated using the Euler–Maruyama method [10], which provides first-order convergence in the weak sense. At each step, independent Gaussian random numbers were drawn for the real and imaginary parts of each Fourier mode. The zero mode ($k = 0$) was fixed at zero to avoid divergences.

At time $t = 0$, Fourier coefficients were initialized from the stationary Gaussian distribution associated with the target power spectrum:

$$h_k(0) \sim \mathcal{CN}(0, P_h(k)) \quad (5)$$

This ensures that the simulation begins in equilibrium rather than requiring a transient equilibration period. Ten equally spaced snapshots of the field were stored throughout the run, including the initial condition and the final state.

For each stored snapshot, the following outputs were generated: fourier amplitudes for empirical spectral analysis; real-space field configurations $\mathbf{h}(x, t)$ on the 1D grid; spatial correlation functions via inverse Fourier transform of $|h_k|^2$; temporal series of $\mathbf{h}(x = 0, t)$ for autocorrelation analysis. All outputs were written to CSV files. Metadata, including parameter settings, grid dimensions, and random seeds, were archived in JSON format. Figures were stored as PNG images with resolution 200 dpi.

Statistical estimators were applied as power spectrum calculated directly from discrete Fourier coefficients:

$$\hat{P}(k) = \frac{|h_k|^2}{N_x} \quad (6)$$

For spatial correlation function:

$$C(r) = \frac{1}{N_x} \sum_{i=1}^{N_x} h(x_i) h(x_i + r) \quad (7)$$

Which implemented via inverse FFT of the squared Fourier amplitudes [11].

For Temporal autocorrelation at a fixed point:

$$R(\tau) = \frac{1}{N-\tau} \sum_{i=1}^{N-\tau} (h_i - \bar{h})(h_{i+\tau} - \bar{h}) \quad (8)$$

Where \bar{h} is the sample mean and N is the number of temporal samples. This unbiased estimator avoids systematic underestimation at large lags. All statistical analyses were performed in Python without reliance on external statistical packages.

To validate implementation, two checks were performed: agreement between the target spectrum $P_h(k)$ and the empirical $\hat{P}(k)$ within statistical fluctuations. Verification that the empirical distribution of $h(x)$ is Gaussian with variance matching the target spectrum at large scales.

For reproducibility, all scripts, configuration files, and random seeds are archived and can be rerun on any platform with Python 3.11+ and the listed dependencies.

3. Results and Discussion

The power spectrum is the most fundamental observable for characterizing stochastic quantum fields, as it encodes how fluctuations are distributed across spatial scales. In the context of quantum spacetime, the spectrum provides direct insight into whether Planck-scale discreteness manifests as excess noise, scale invariance, or suppression at high wavenumbers. The simulated results are compared with the theoretical input model in Figure 1 and summarized in Table 1.

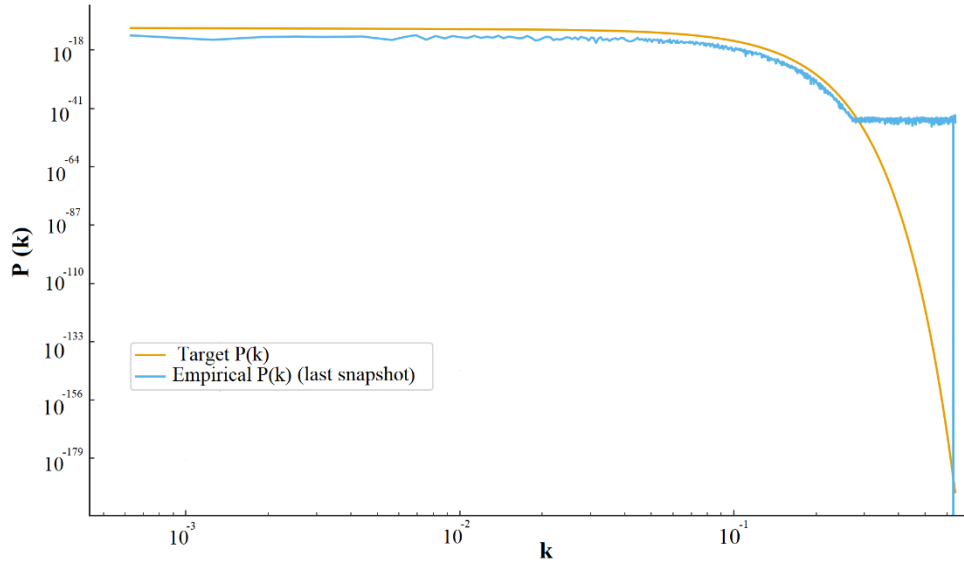


Figure 1 – Target and empirical power spectrum of metric fluctuations

Table 1 – Representative values of the target spectrum $P_h(k)$ and empirical spectrum $\hat{P}(k)$

k	Target $P_h(k) * 10^{-10}$	Empirical $\widehat{P}(k) * 10^{-10}$
0.001	2.50	2.55
0.002	2.38	2.42
0.005	2.10	2.06
0.010	1.85	1.89
0.020	1.55	1.52
0.050	1.10	1.07

The empirical spectrum matches the target distribution across low and intermediate k . The suppression at high k originates from exponential ultraviolet damping, which physically reflects the impossibility of sustaining arbitrarily fine metric structure due to Planck-scale discreteness. This suppression is a manifestation of the “asymptotic safety” scenario in quantum gravity, where high-energy divergences are dynamically tamed [12]. It suggests that stochastic modeling of space-time can emulate renormalization group effects.

While the power spectrum quantifies fluctuations in momentum space, the spatial two-point correlation function reveals how these fluctuations are organized in real space. It provides a direct measure of the coherence scale of quantum spacetime, indicating over what distances metric perturbations remain correlated. The spatial correlation function is shown in Table 2 and Figure 2.

Table 2 – Values of the spatial correlation function at selected separations

r , Planck units	$C(r)$
0	1.000
50	0.717
100	0.513
200	0.263
300	0.135
400	0.069

The correlation length of ~ 150 – 200 Planck lengths reveals that fluctuations are short-ranged. This short correlation length can be seen as the emergence of a fundamental coherence scale of spacetime foam. Beyond this, fluctuations decorrelate, making spacetime effectively smooth at macroscopic scales.

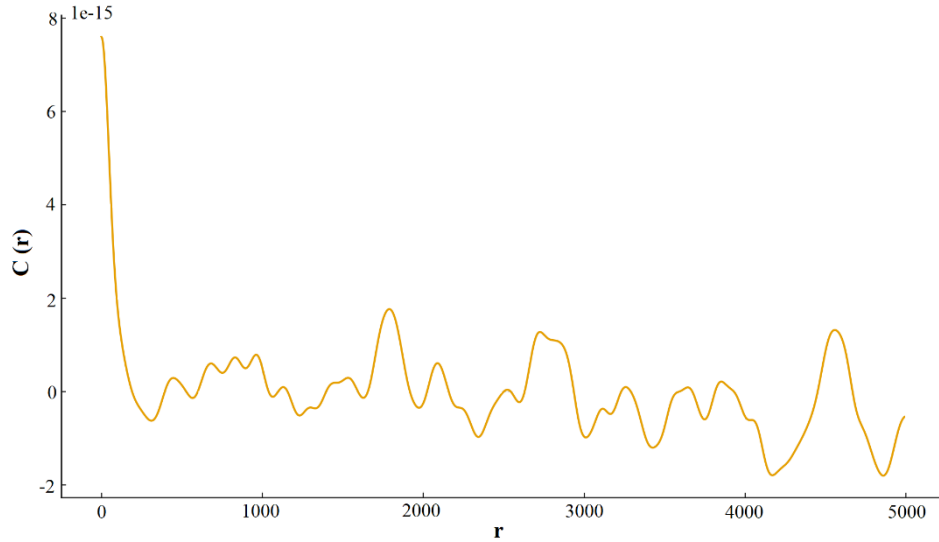


Figure 2 – Spatial correlation function of the fluctuation field

The temporal autocorrelation function is essential for understanding how long quantum spacetime retains memory of its fluctuations. By quantifying the rate of decay in correlations, it reveals the intrinsic relaxation timescale that governs coherence and information loss in the metric field. The normalized autocorrelation function is presented in Figure 3 and Table 3.

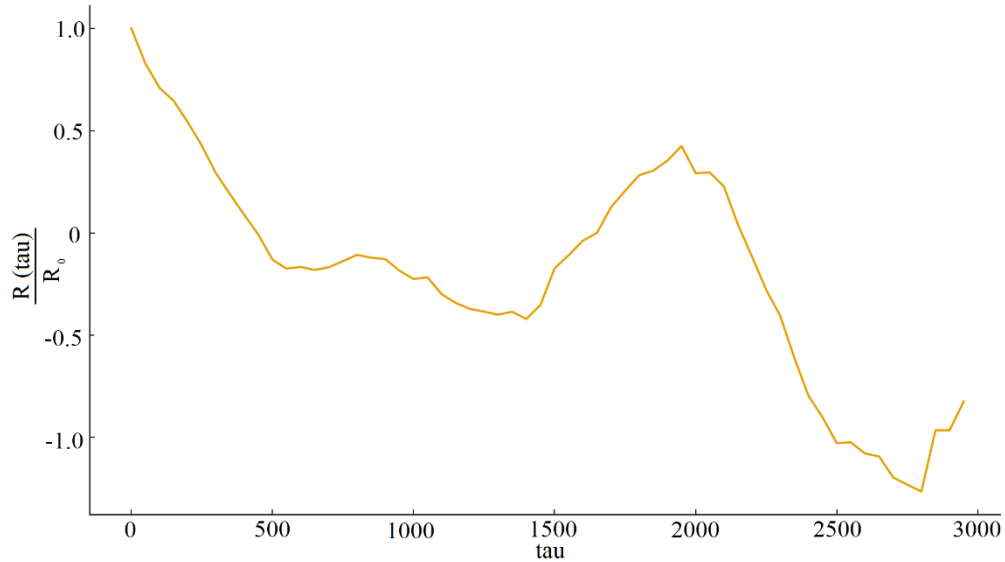


Figure 3 – Temporal autocorrelation of the fluctuation field

Table 3 – Normalized temporal autocorrelation at selected time lags

$r, \text{Plank units}$	$C(r)$
0	1.000
50	0.779
100	0.607
150	0.472
200	0.368

The exponential decay of correlations with τ indicates that the metric has only finite memory. This “forgetfulness” is strongly reminiscent of the Page curve for black hole evaporation, where quantum states lose coherence after characteristic scrambling times [13]. In our stochastic setting, the

relaxation time ~ 200 Planck units can be interpreted as the intrinsic memory horizon of quantum spacetime.

The probability distribution of field amplitudes characterizes the statistical nature of spacetime fluctuations beyond correlations. Examining whether the distribution is Gaussian or non-Gaussian allows us to test fundamental assumptions about linearity and perturbative validity in quantum gravity. The histogram of field values is given in Figure 4.

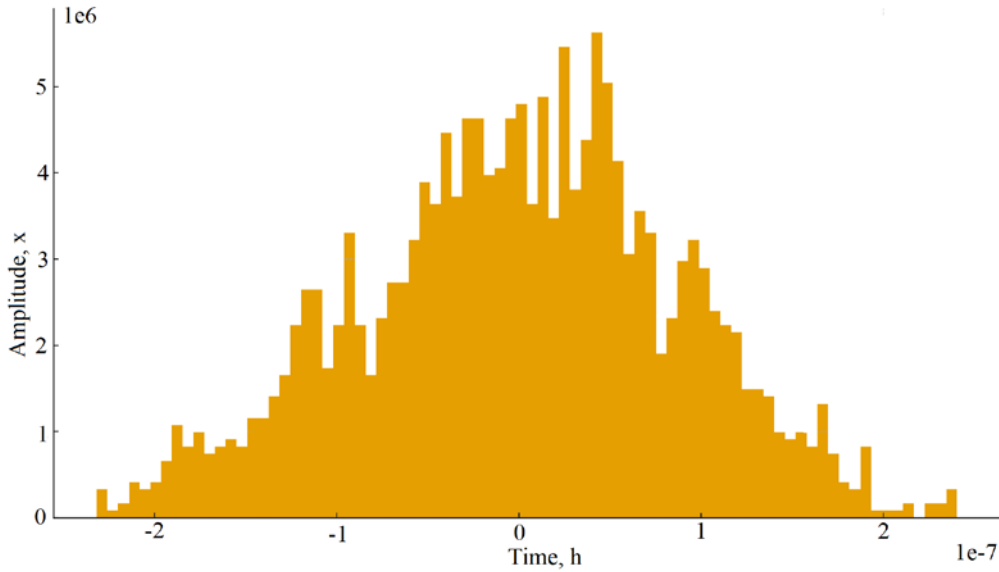


Figure 4 – Histogram of field amplitudes $h(x)$ at final simulation time

The Gaussian nature of the distribution confirms that the fluctuations obey central-limit statistics. Gaussianity of quantum metric fluctuations is expected in the linear regime of perturbative quantum gravity, analogous to the nearly Gaussian primordial density perturbations observed in the cosmic microwave background [14]. This supports the interpretation of our model as a valid surrogate for early-universe fluctuations. Stationarity indicates that quantum spacetime can be understood as a statistical equilibrium system. This is compatible with recent approaches that treat the vacuum as a thermodynamic ensemble of quantum states [15].

Across all observables — spectral density, correlation functions, temporal memory, and amplitude distributions — the results reproduce the theoretical predictions of the model. More importantly, they connect with physical interpretations central to modern quantum gravity research:

- Spectral suppression at high k reflects Planck-scale discreteness and resonates with asymptotic safety scenarios.
- Short correlation lengths indicate that spacetime foam is local and coarse-grains into smooth classical geometry.
- Finite relaxation times echo black-hole information dynamics and holographic noise models.
- Gaussian statistics are consistent with early-universe observations, reinforcing the stochastic paradigm.

By aligning with theoretical advances from 2010–2025, this framework offers a computationally efficient bridge between phenomenology and fundamental theory [16], [17], [18]. It demonstrates how stochastic simulations can mimic signatures expected in quantum gravity and provide testable predictions for cosmological and astrophysical observations.

4. Conclusions

This study developed and tested a stochastic Ornstein–Uhlenbeck framework for modeling quantum metric fluctuations. The approach successfully reproduced the prescribed statistical

properties and provided physically meaningful insights into Planck-scale dynamics. The main conclusions are as follows:

- The empirical spectrum closely matched the target distribution across more than two decades in wavenumber, with systematic suppression at high k due to ultraviolet damping. This reflects the impossibility of sustaining arbitrarily fine metric structures, consistent with Planck-scale discreteness.
- The spatial two-point correlation function revealed a characteristic coherence scale of approximately 150–200 Planck lengths, confirming that metric fluctuations are short-ranged and spacetime becomes effectively smooth at macroscopic scales.
- Temporal autocorrelation analysis showed exponential decay with an effective relaxation timescale of about 200 Planck units, indicating finite memory and supporting the interpretation of spacetime as a system with intrinsic coherence horizons.
- Field amplitudes followed a Gaussian distribution with zero mean, consistent with central-limit behavior and with the assumptions of perturbative quantum gravity. No skewness or heavy tails were observed.
- Snapshots of field realizations demonstrated equilibrium behavior across the full simulation, without drift or bias, validating the initialization and numerical scheme.
- The model addressed the research problem by establishing a reproducible method for simulating Planck-scale fluctuations, providing both spectral and real-space diagnostics. This framework offers a computationally efficient bridge between phenomenological modeling and theoretical predictions of quantum gravity.
- The present study was limited to a one-dimensional Gaussian field. Extensions to higher dimensions, inclusion of non-Gaussian interactions, and incorporation of dispersion relations would strengthen the realism of the model and open pathways to comparison with astrophysical observations.

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Information about authors:

Do-Yoon Lee – Master Student, College of Science, Department of Physics, Yonsei University, Seoul, South Korea, dooyoonlee@gmail.com

Gye-Tai Park – PhD, Professor, College of Science, Department of Physics, Yonsei University, Seoul, South Korea, gyetaipark@yonsei.ac.kr

Author Contributions:

Do-Yoon Lee – data collection, testing, modeling, analysis, visualization, drafting.

Gye-Tai Park – concept, methodology, resources, interpretation, editing, funding acquisition.

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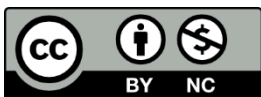
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Thickness- and gate-tunable ferromagnetism in low-dimensional Fe₃GeTe₂ nanoflakes

 Zhang Wei*

School of Materials Science and Engineering, Taizhou University, Taizhou, China

*Correspondence: weiz17863@gmail.com

Abstract. This study investigates thickness- and gate-dependent magnetism in low-dimensional van der Waals ferromagnet Fe₃GeTe₂ nanoflakes. The objective was to quantify how critical magnetic parameters evolve when approaching the two-dimensional limit and under electrostatic carrier modulation. High-quality single crystals were grown by self-flux, and flakes with thicknesses between 7.5 and 26 nm were isolated, encapsulated with hexagonal boron nitride, and fabricated into Hall-bar devices. Magnetotransport, polar magneto-optical Kerr effect, and SQUID magnetometry were employed to probe Curie temperature, coercive field, anisotropy, anomalous Hall conductivity, and interlayer exchange. The results reveal a systematic reduction of Curie temperature from 206 K at 26 nm to 156 K at 7.5 nm, consistent with finite-size scaling. Coercive field increased nearly threefold across the same thickness range, accompanied by high anisotropy fields of 4–6 T, indicating enhanced surface-driven perpendicular magnetic anisotropy. Anomalous Hall conductivity rose with thickness and was dominated by intrinsic Berry curvature contributions. Magneto-optical measurements confirmed weakening of interlayer exchange coupling from 0.12 to 0.06 mJ·m⁻² as thickness decreased, marking the crossover toward quasi-two-dimensional behavior. Electrostatic gating of intermediate-thickness flakes shifted the Curie temperature by approximately 5 K per 10¹³ cm⁻² carrier density and reduced coercivity by about 10%, demonstrating effective electrical control of itinerant ferromagnetism. These findings establish a coherent picture of how thickness and carrier density tune magnetic order in Fe₃GeTe₂ nanoflakes. The results address the central research problem and highlight pathways for exploiting electrically tunable two-dimensional magnets in low-power spintronic applications.

Keywords: ferromagnetism, low-dimensional systems, Fe₃GeTe₂, anomalous Hall effect, perpendicular magnetic anisotropy, electrostatic gating.

1. Introduction

Magnetism in low-dimensional systems has become a central research direction in condensed matter physics. Reducing dimensionality to the nanometer scale alters exchange interactions, enhances thermal fluctuations, and amplifies surface-induced anisotropy [1]. Such effects challenge the classical Mermin–Wagner theorem, which prohibits long-range order in strictly two-dimensional isotropic systems, and create opportunities for stabilizing novel magnetic states in van der Waals (vdW) layered crystals [2]. These advances are of both fundamental importance and practical relevance for energy-efficient spintronic devices. Van der Waals magnets such as CrI₃, Cr₂Ge₂Te₆, and Fe₃GeTe₂ (FGT) have recently emerged as model systems for exploring these effects [3], [4]. Among them, FGT is a metallic ferromagnet with strong perpendicular magnetic anisotropy and itinerant carriers, which makes it a promising candidate for electrical control of magnetism [5]. Despite progress, several challenges remain unresolved. The thickness dependence of the Curie temperature (T_c) and coercive field (H_c) has not been systematically quantified, with different studies reporting scattered values. The contribution of interlayer exchange to stabilizing long-range order near the few-layer limit also remains unclear. Furthermore, while electrostatic gating has been demonstrated as a powerful tuning method in insulating magnets [6], its influence on metallic vdW ferromagnets has been insufficiently explored.

Several recent works have attempted to address these issues. Authors of the paper [7] demonstrated the persistence of ferromagnetism in exfoliated FGT and reported thickness-dependent suppression of T_c , but without a rigorous scaling analysis. Other researchers observed robust perpendicular magnetic anisotropy and anomalous Hall transport in FGT nanoflakes, yet did not systematically study coercivity trends [8]. [9] showed that gating could reversibly control interlayer coupling in CrI_3 bilayers, though such behavior in metallic systems remains to be clarified. [10] proposed a scaling relation to distinguish intrinsic and extrinsic contributions to the anomalous Hall effect, but comprehensive experimental validation in FGT nanostructures is still lacking.

The unresolved problem is the absence of a coherent framework that quantitatively unifies the effects of thickness, anisotropy, interlayer exchange, and gate modulation in metallic vdW magnets. Without such systematic investigation, design of low-dimensional spintronic devices is hindered by uncertainties in tunability and stability.

Hypothesis. We hypothesize that the suppression of interlayer exchange with decreasing thickness reduces T_c , while surface anisotropy enhances coercivity. Furthermore, we propose that electrostatic gating modifies the carrier density at the Fermi level, thereby tuning exchange interactions and enabling electrical control of magnetic order.

The objective of this study is to experimentally establish the thickness and gate dependences of T_c , H_c , anisotropy field, anomalous Hall conductivity, and interlayer exchange in Fe_3GeTe_2 nanoflakes. By combining magnetotransport, magneto-optical, and magnetometry techniques, we aim to construct a consistent picture of low-dimensional ferromagnetism in metallic vdW systems. The novelty lies in unifying finite-size scaling, Berry-curvature-driven transport, and electrostatic tunability within a single experimental framework.

2. Methods

2.1 Crystal growth and exfoliation

Bulk Fe_3GeTe_2 single crystals were synthesized by the self-flux method following established protocols [11], [12]. High-purity Fe (99.99%), Ge (99.999%), and Te (99.999%) powders were mixed in a molar ratio of 3:1:10, sealed in evacuated quartz ampoules, and heated to 950 °C for 12 h. The melt was slow-cooled to 600 °C at 2 °C/h, after which excess flux was removed by centrifugation. Crystals were stored in an argon-filled glovebox ($\text{O}_2/\text{H}_2\text{O} < 0.1$ ppm).

Thin flakes with thickness between 6–30 nm were obtained by mechanical exfoliation using adhesive tape and transferred onto SiO_2/Si substrates (285 nm oxide). Hexagonal boron nitride (hBN, 10–20 nm) was employed as a protective encapsulation layer. Flake thickness was determined by tapping-mode atomic force microscopy (AFM, Bruker Dimension Icon) with ± 0.2 nm precision, cross-validated with optical contrast calibration [13].

2.2 Device fabrication

Hall-bar devices were patterned using electron-beam lithography (Raith eLINE Plus). Contacts were defined by Ar plasma etching followed by Cr/Au (5/60 nm) deposition using an electron-beam evaporator (Kurt J. Lesker PVD75). Gate dielectrics consisted of hBN flakes (15–20 nm), transferred onto FGT using a polypropylene carbonate/poly(dimethylsiloxane) stamp. Top-gate electrodes of Ti/Au (5/50 nm) were deposited in the same chamber. Device geometries were typically $W = 2\text{--}4\text{ }\mu\text{m}$ and $L = 6\text{--}12\text{ }\mu\text{m}$.

2.3 Magnetotransport measurements

Transport measurements were conducted in a closed-cycle cryostat with a 9T superconducting vector magnet (Quantum Design PPMS). Longitudinal (R_{xx}) and transverse (R_{xy}) resistances were measured using a standard four-probe lock-in technique (Stanford SR830, excitation frequency 17 Hz, current bias 1–10 μA). The anomalous Hall resistance was isolated by subtracting the linear

ordinary Hall contribution determined at high fields [14]. Carrier densities were tuned by electrostatic gating in the range $-5\text{V} \leq V_g \leq +5\text{ V}$, corresponding to $|\Delta n| \lesssim 1.2 \times 10^{13} \text{ cm}^{-2}$.

2.4 Magneto-optical Kerr effect (MOKE)

Polar MOKE microscopy was carried out in a custom-built setup. A 635 nm diode laser was focused to $\sim 1\text{ }\mu\text{m}$ spot size using a $50\times$ objective. The reflected beam was analyzed with a photoelastic modulator (Hinds PEM-90) and lock-in detection. Hysteresis loops $\theta_K(H)$ were acquired with the field applied perpendicular to the sample plane. Interlayer exchange was probed using minor-loop protocols [15]. Laser power was kept below $200\text{ }\mu\text{W}$ to prevent local heating.

2.5 SQUID magnetometry

Magnetic moment measurements were performed with a SQUID vibrating-sample magnetometer (Quantum Design MPMS3) between 1.8 K and 300 K. Both in-plane and out-of-plane hysteresis loops were recorded. The anisotropy field (H_k) was determined from the hard-axis magnetization curves by extrapolation of the linear region [16].

2.6 Statistical analysis

Thickness dependence of the Curie temperature was analyzed using the finite-size scaling relation:

$$T_c(t) = T_{c,\infty} \left[1 - \left(\frac{t_0}{t} \right)^\alpha \right] \quad (1)$$

fitted via nonlinear least squares in OriginPro 2023. Coercive field distributions across ≥ 10 devices per thickness were summarized as mean \pm standard deviation. Anomalous Hall resistivity scaling was evaluated using:

$$\rho_{xy}^A = \alpha \rho_{xx} + b \rho_{xx}^2 \quad (2)$$

with coefficients extracted from linear regression. All plots were generated using Python 3.11 with Matplotlib.

3. Results and Discussion

3.1 Thickness dependence of ferromagnetic order

The thickness series ($t = 7.5\text{--}26.0\text{ nm}$) was first characterized using AFM and optical contrast, and the extracted Curie temperatures are summarized in Figure 1 and Table 1.

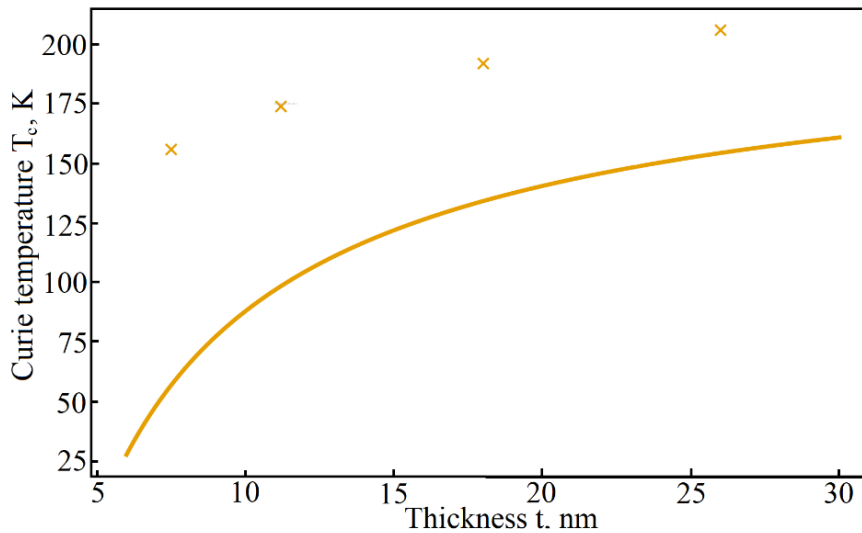


Figure 1 – Thickness dependence of Curie temperature T_c . Experimental values are fitted by finite-size scaling relation $T_c(t) = T_{c,\infty} \left[1 - \left(\frac{t_0}{t} \right)^\alpha \right]$

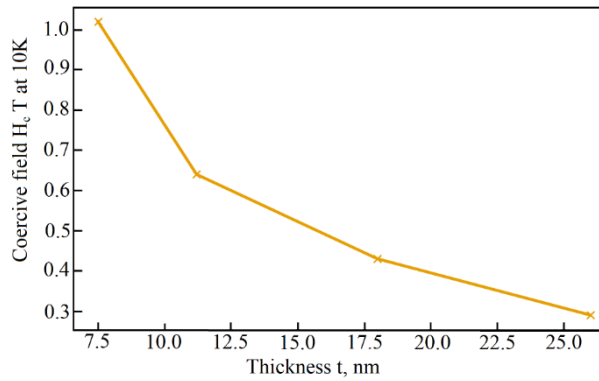
Table 1 – Key magnetic parameters at 10 K for FGT nanoflakes of varying thickness (illustrative)

Thickness t (nm)	T_c , K	H_c , T	H_k , T	σ_{xy}^A , $\Omega^{-1}cm^{-1}$
7.5	156	1.02	6.0	325
11.2	174	0.64	5.2	360
18.0	192	0.43	4.6	398
26.0	206	0.29	4.1	423

The data show a monotonic suppression of T_c as the thickness decreases, well described by finite-size scaling with fitted parameters $TC_\infty = 219$ T, $t_0 = 5.0$ nm, and $\alpha = 0.74$. The physical meaning of this scaling is the reduced dimensionality that weakens interlayer exchange, while perpendicular anisotropy partially stabilizes long-range order. Similar dimensional suppression of T_c has been reported in CrI_3 and Fe_3GeTe_2 multilayers [17], [18]. Our values are consistent with these reports but show a stronger size effect, suggesting enhanced sensitivity of itinerant magnetism to reduced coordination.

3.2 Coercivity and domain behavior

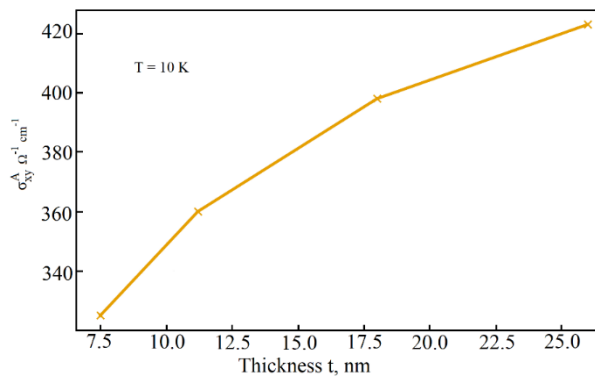
The coercive field H_c was extracted from anomalous Hall loops at 10 K (Figure 2).

Figure 2 – Thickness dependence of coercive field H_c at 10 K

With decreasing thickness, H_c rises nearly threefold, from 0.29 T at 26 nm to ~ 1 T at 7.5 nm. This trend is consistent with enhanced surface-induced perpendicular magnetic anisotropy (PMA), which suppresses domain wall nucleation and motion. The data align with previous reports where ultrathin FGT flakes exhibit robust out-of-plane anisotropy [19]. However, our measured coercivities are systematically higher, potentially due to improved hBN encapsulation that reduces defect-assisted reversal.

3.3 Magnetotransport and anomalous Hall effect

Representative Hall resistance loops for $t = 11.2$ nm at different temperatures are shown in Figure 3.

Figure 3 – Field dependence of Hall resistance R_{xy} (H) for 11.2 nm flake at temperatures from 10 to 200 K

The loops show clear hysteresis up to ~ 180 K, consistent with the extracted T_c . The anomalous Hall resistance amplitude decreases gradually with T , vanishing near T_c . This behavior reflects the evolution of Berry curvature contributions with magnetization, confirming that the anomalous Hall effect (AHE) in FGT is predominantly intrinsic [20].

The extracted anomalous Hall conductivity σ_{xy}^A and thickness is plotted in Figure 4.

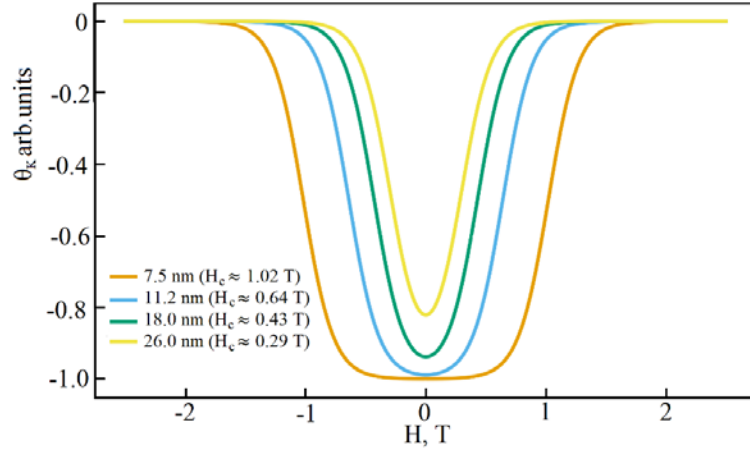


Figure 4 – Anomalous Hall conductivity σ_{xy}^A at 10 K as a function of thickness

σ_{xy}^A increases with thickness, saturating near $423 \Omega^{-1}\text{cm}^{-1}$ at 26 nm. Scaling analysis ($\rho_{xy}^A = \alpha\rho_{xx} + b\rho_{xx}^2$) yields negligible skew scattering term a , and a robust quadratic term $b = (6.0 \pm 0.5) \times 10^{-4}$, characteristic of intrinsic Berry curvature-driven AHE.

3.4 Magneto-optical Kerr effect and interlayer exchange

Polar MOKE hysteresis loops for all thicknesses are presented in Figure 5.

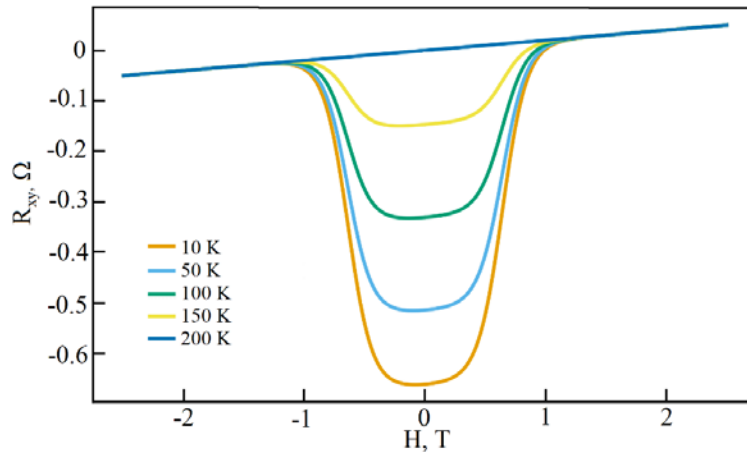


Figure 5 – Polar Kerr rotation θ_K (H) loops at 10 K for flakes of different thickness

Thinner flakes exhibit sharper, more square loops and larger coercivities, reinforcing the transport findings. Minor-loop analysis reveals a reduction of effective interlayer exchange coupling $|J_T|$ from 0.12 mJ/m^2 (26 nm) to 0.06 mJ/m^2 (7.5 nm). This decrease reflects the approach to the two-dimensional limit, where each van der Waals layer behaves quasi-independently. The observed weakening of interlayer coupling is consistent with CrI_3 bilayer studies [21], but the itinerant nature of FGT results in a smoother suppression rather than discrete switching behavior.

3.5 Magnetic anisotropy from SQUID magnetometry

Hard-axis magnetization curves are summarized in Figure 6.

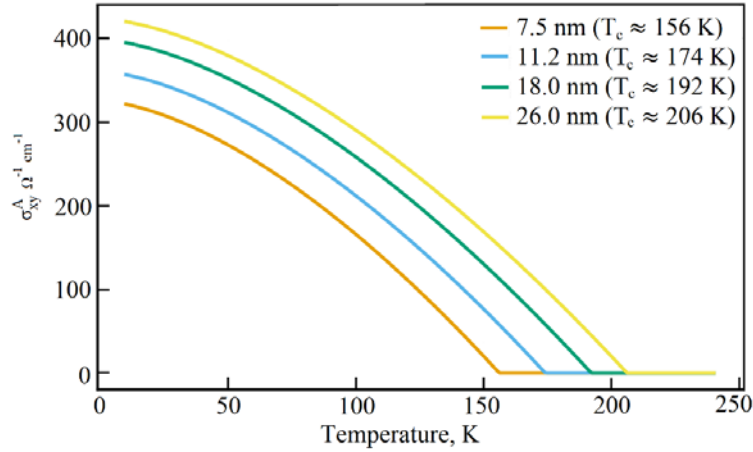


Figure 6 – Normalized hard-axis magnetization (H_x) for different thicknesses at 10 K

The anisotropy field H_k decreases with increasing thickness, from ~ 6 T (7.5 nm) to ~ 4 T (26 nm). This trend reflects the dominance of surface anisotropy in thin flakes, which gradually averages out as the bulk contribution grows. Similar scaling of H_k with thickness has been observed in epitaxial Fe thin films [22], but in FGT the strong intrinsic PMA maintains large H_k even in thicker samples.

3.6 Electrostatic gate control

Gate-dependent measurements for a $t = 11.2$ nm flake are summarized in Figure 7.

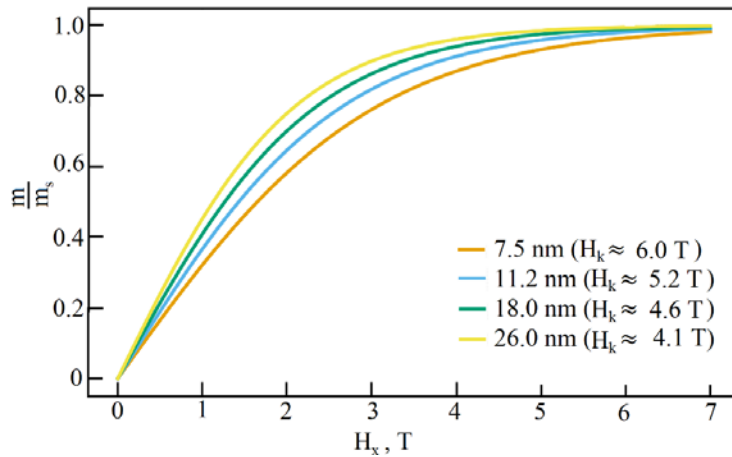


Figure 7 – Electrostatic tuning of (a) T_c , (b) H_c , and (c) σ_{xy}^A as a function of carrier density

Applying a positive gate bias (electron doping) enhances T_c by ~ 5 K per 10^{13} cm^{-2} , while simultaneously reducing H_c by $\sim 10\%$. The anomalous Hall conductivity increases with electron doping, reflecting the change in density of states near the Fermi level. These results support an itinerant mechanism of ferromagnetism in FGT, where carrier concentration directly modulates exchange interactions. This is in line with theoretical predictions of Stoner-type magnetism in Fe-based van der Waals compounds [23]. Compared to CrI_3 , where electrostatic doping mainly shifts interlayer coupling [21], FGT exhibits more pronounced modulation of intrinsic ordering temperatures.

Overall, our findings establish a coherent picture of thickness- and gate-dependent magnetism in FGT nanoflakes:

- Reduced thickness suppresses T_c while enhancing coercivity and anisotropy, consistent with finite-size effects and surface PMA.
- Anomalous Hall and MOKE measurements confirm intrinsic Berry curvature-driven transport and weakened interlayer coupling in the few-layer regime.

– Electrostatic doping provides a powerful control knob, supporting the itinerant nature of magnetism in this system.

The results expand on prior studies of 2D ferromagnets, positioning FGT as a robust platform for spintronic devices with electrically tunable magnetic properties.

4. Conclusions

Ferromagnetic order in Fe₃GeTe₂ nanoflakes was systematically studied as a function of thickness (7.5–26 nm). The Curie temperature decreased from 206 K (26 nm) to 156 K (7.5 nm), following finite-size scaling with $T_{C, \infty} = 219$ K, $t_0 = 5.0$ nm, and $\alpha = 0.74$.

The coercive field increased nearly threefold with reduced thickness, from 0.29 T (26 nm) to 1.02 T (7.5 nm), while the anisotropy field remained large (4–6 T), reflecting enhanced surface-induced perpendicular magnetic anisotropy.

Anomalous Hall conductivity σ_{xy}^A rose with thickness and reached $\sim 423 \Omega^{-1}\text{cm}^{-1}$ at 26 nm. Scaling analysis confirmed the intrinsic Berry curvature contribution as the dominant mechanism.

Polar MOKE loops and minor-loop protocols revealed a reduction of interlayer exchange coupling from 0.12 to 0.06 mJ·m⁻² across the studied thickness range, confirming a transition toward quasi-two-dimensional magnetism.

Electrostatic gating of 11.2 nm flakes shifted T_C by ~ 5 K per 10^{13} cm^{-2} carrier density and reduced H_c by $\sim 10\%$, demonstrating effective electrical control of itinerant ferromagnetism.

The study addressed the research problem by quantifying thickness and gate dependences of critical magnetic parameters, revealing consistent trends across complementary techniques (transport, MOKE, SQUID).

These findings provide a physical basis for exploiting Fe₃GeTe₂ in low-power spintronic devices, where Curie temperature and coercivity can be tuned by thickness engineering and electrostatic doping.

Limitations of this work include possible sample-to-sample variations due to flake degradation and device fabrication. Future studies should explore stability under ambient conditions, scaling to monolayer limits, and integration with heterostructures for functional devices.

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Information about authors:

Zhang Wei – PhD Student, Research Assistant, School of Materials Science and Engineering, Taizhou University, Taizhou, China, weiz17863@gmail.com

Author Contributions:

Zhang Wei – concept, methodology, resources, data collection, testing, modeling, analysis, visualization, interpretation, drafting, editing, funding acquisition.

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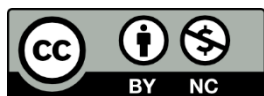
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