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Synergistic Integration of MEMS and Spintronics for Precision Data Analytics in Cheminformatics

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Abstract

The transformative potential of merging spintronics and micro-electromechanical systems (MEMS) technologies in cheminformatics is investigated in this work. Recent advancements in MEMS, particularly through the use of microbeam sensors and accelerometers, have enhanced the precision of data collection and processing, especially in biomedical applications such as drug delivery systems and chemical sensing. The synchronization of oscillations in MEMS devices leads to improved reliability and data accuracy, thereby enabling the development of sophisticated cheminformatics models. Meanwhile, spin-torque nano-oscillators (STNOs) present a groundbreaking method for generating tunable microwave signals, which could significantly enhance signal-processing capabilities in cheminformatics. Their low power consumption and compatibility with complementary metal-oxide-semiconductor (CMOS) technology make STNOs ideal for applications in molecular sensors and data-logging systems. This paper elucidates the synergistic benefits of these technologies in facilitating real-time data transmission and analysis, ultimately advancing predictive modeling and cheminformatics databases.

Keywords: Biomedical applications, cheminformatics, micro-electromechanical systems (MEMS), data processing, spin-torque nano-oscillators (STNOs), spintronics

INTRODUCTION

The rapid evolution of nanoscale technologies has significantly impacted various scientific fields, with cheminformatics standing at the forefront of these advancements. Cheminformatics integrates chemistry, computer science, and information technology to enhance our understanding of chemical compounds and their interactions. As the demand for precise data and real-time analysis in cheminformatics continues to grow, the exploration of innovative technologies becomes increasingly essential.

Micro-electromechanical systems (MEMS) have emerged as pivotal tools in this domain, particularly due to their ability to provide high-resolution sensing and actuation capabilities. The use of MEMS-based microbeam sensors and accelerometers facilitates the synchronization of oscillations, leading to enhanced data-collection methodologies. These advancements are particularly valuable in biomedical applications, where precise dosage control in drug delivery systems is critical. The incorporation of MEMS technology not only improves the reliability of measurements but also enhances the overall functionality of devices used in chemical sensing [1].

Concurrently, spintronics technology, particularly through the development of spin-torque nano-oscillators (STNOs), offers new possibilities for generating microwave signals with tunable

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frequencies. STNOs operate with low power requirements and are compatible with existing CMOS technologies, making them suitable candidates for integration into molecular sensors and data-logging systems. The ability to generate tunable microwave signals facilitates improved signal processing in cheminformatics applications, particularly in real-time data transmission and analytics.

This paper aims to explore the integration of MEMS and spintronics technologies in cheminformatics, highlighting their respective roles in enhancing the precision and functionality of nanoscale devices. By leveraging the unique properties of these technologies, we propose a pathway for significant advancements in sensor integration, data collection, and real-time processing. The synergy between MEMS and spintronics holds promise for the future of cheminformatics, paving the way for more accurate predictive modeling and advanced chemical informatics databases [2, 3].

MICROBEAM SENSOR-COUPLED MEMS ACCELEROMETER

This study focuses on synchronizing oscillations of weakly coupled microbeam elements in a differential resonant MEMS accelerometer operating in dual-loop self-oscillator mode. The multiscale method is employed to analyze a system of two Van der Pol self-oscillators with nonlinear elastic coupling, modeled using the Galerkin method. Both analytical and numerical approaches reveal beat modes and synchronization between the two resonators, with boundaries in the system parameter space. Global analysis and local bifurcation studies show coexistence zones of stable synchronization and beat modes, including their basins of attraction. These parametric zones are influenced by the inherent or designed nonidentity of the resonators.

Beam Deflection Oscillation Effects on Weld Geometry

Electron beam welding with local beam deflection oscillations affects seam profiles and heat-affected zones. Experimental results demonstrate minimal control over the beam cross-sectional profile based on welding velocity, focus position, and beam power. Significant changes occur only when the beam focus is 18 mm below the weld surface, with longitudinal oscillations related to workpiece movement, enhancing weld root radius and eliminating spiking. Other focus positions produced dagger-like cross-sections. Beam self-focusing on the keyhole's lower part explains minimal oscillation effects on the weld root shape. Statistical analysis of geometric parameters highlights that maximum weld depths occur at focusing currents of 840–850 mA with longitudinal oscillations at 745 Hz. The dynamic power distribution around the beam's stationary position is affected by deflection oscillations. Despite advancements in electron beam welding, understanding the influence of beam oscillation frequency, trajectory, and amplitude remains incomplete and sometimes contentious [4, 5].

Nano/Micro-Beam Investigation Based on Deflections

Micro- and nano-beam MEMS devices are critical for precision mechanical motion and small-scale sensing. This study examines the impact of axial forces on MEMS device deflection, especially in biomedical applications like drug delivery systems. Using the Galerkin method, the nonlinear equation for a doubly clamped beam under van der Waals (vdW) force is solved. The homotopy perturbation method (HPM) and Akbari Ganji Method (AGM) are applied, with results validated against the Runge-Kutta method. The impact of compressive and tensile axial forces on beam deflection is analyzed, showing increased deflection in compressive modes and the opposite trend in tensile modes. The study highlights the importance of understanding vdW forces, even though they are weak, for optimizing the design and performance of nanoscale and microscale devices, particularly MEMS sensors and actuators [6].

Pull-in instability in electrostatically actuated MEMS is also addressed, with a focus on how increasing input voltage beyond critical thresholds influences behavior. Applications in drug delivery are particularly noteworthy, where MEMS microbeams allow precise dosage control and spatial drug release. Several analytical methods, including AGM and HPM, are applied to solve nonlinear equations governing the behavior of MEMS under vdW forces. These methods offer accurate solutions, advancing the design and application of MEMS in areas like drug delivery, telecommunication devices, and materials engineering.

Voltage and Current-Free Spin-Transfer Nano-Oscillator

Spin-transfer nano-oscillators (STNOs) generate microwave signals by transferring spin angular momentum through spin-polarized currents. However, their reliance on external magnetic fields and high drive currents has limited their practical applications due to issues related to size and power dissipation. In this study, we report microwave measurements on STNOs constructed with MgO-based magnetic tunnel junctions (MTJs), featuring a perpendicular free layer and planar polarizer. These STNOs demonstrate high-output-power microwave emission at ultralow current densities without the need for bias magnetic fields. The critical current density observed is more than an order of magnitude smaller than previously reported. These findings suggest that STNOs could enhance integration with complementary metal-oxide-semiconductor (CMOS) technology, opening new possibilities for the development of on-chip oscillators [7, 8].

Oscillators, fundamental to numerous communication, navigation, and measurement systems, provide periodic output for various applications, such as generating electromagnetic energy, enabling frequency conversion, and performing clocking functions in digital systems. STNOs are promising for on-chip integration due to their frequency tunability, nanoscale size, wide operating temperature range, and compatibility with CMOS technology. However, challenges remain in optimizing their dynamic characteristics, including high-frequency operation, narrow spectral linewidth, and operation without external magnetic fields or high current densities.

One key component in improving STNOs is interfacial perpendicular anisotropy (IPA) between ferromagnetic electrodes and the MTJ tunnel barrier, typically achieved with CoFeB/MgO materials. IPA has been used to either reduce out-of-plane demagnetizing fields or align magnetizations in-plane. Here, we balance IPA and the out-of-plane demagnetizing field to design STNOs with an asymmetric MTJ structure. This configuration enhances large-angle free layer precession, resulting in high output power without a bias magnetic field. The primary technological challenges addressed are reducing the need for external bias fields and lowering drive current densities, both of which are critical for reducing power dissipation and enabling the use of smaller transistors in CMOS-integrated oscillators [9].

Spin-Torque Nano-Oscillator

STNOs, which rely on spin-transfer torque (STT) from spin-polarized currents, are highly tunable microwave generators with applications in neuromorphic computing and frequency signal generation. Typically composed of MTJ stacks with nanofabricated geometries, STNOs have faced challenges due to the high currents required for auto-oscillations, which can cause device damage. STT-driven oscillations occur when spin current compensates for Gilbert damping in the free layer. In this study, we use spin injection mechanisms, including spin polarization and the spin Hall effect, to excite a 3-terminal STNO. This hybrid excitation leads to increased output power, with critical spin current densities observed at 4.52 ± 0.18 × 10^9 ħ/2 e−1 Am−2. The results highlight the potential of STNOs for microwave generation and other applications requiring precise frequency control.

Spin Current Oscillations in Ferromagnets

Spin current, a fundamental aspect of spintronics, typically decays monotonically during diffusion in materials. However, when a ferromagnet hosts the spin current, spatial oscillations are predicted. This phenomenon was observed in Ni=YIG bilayers through the inverse spin Hall effect, with spin current oscillations detected in nickel films. These oscillations align with theoretical predictions based on Fermi wave vector differences between majority and minority carriers. The results uncover new aspects of spin transport dynamics and offer insights for future spintronic device development.

Microwave Generation by Spin-Transfer Nano-Oscillators

STNOs have garnered significant attention due to their frequency tunability, nanoscale size, wide temperature range, and compatibility with silicon technology. Recent advances in STNO design, particularly those incorporating perpendicular anisotropy, have improved output power towards the microwatt range. Spin-transfer torque-based methods allow magnetic configurations to be altered using spin-polarized currents, leading to persistent precession or reversal of magnetization. STNOs, with their adjustable oscillation frequency and small size, offer advantages over conventional LC-tank voltage-controlled oscillators (VCOs), operating at low voltages and wide temperature ranges. These properties make STNOs suitable for applications such as microwave signal processors, nanosensors, on-chip clocks, and wireless communications.

Theoretical analysis of STNO performance, including frequency, output power, linewidth, and phase noise, continues to evolve. While numerous parameters affect performance, recent developments suggest that STNOs hold great promise for a variety of high-frequency applications in next-generation electronics.

Spin-Orbit Torque Nano-Oscillator: A Breakthrough in Microwave Signal Generation

High-intensity spin wave auto-oscillations, generated at the nanoscale by spin torque and spin Hall effect-based nano-oscillators, are paving the way for novel microwave applications in fields such as spintronics, magnonics, and neuromorphic computing. These devices traditionally rely on externally produced spin currents, either from materials with high spin Hall angles or additional ferromagnetic layers. In this study, we present highly coherent, field- and current-tunable microwave signals originating from nano-constrictions in a single permalloy layer interfaced with oxides, having a thickness of 15–20 nm.

Through a combination of micromagnetic simulations, scanning micro-Brillouin light scattering (BLS) microscopy, and spin-torque ferromagnetic resonance (ST-FMR) measurements, we identify a localized edge mode within the nanoconstriction as the source of auto-oscillations. These oscillations are driven by spin-orbit torques, predominantly arising from the oxide interfaces. Our findings point to significantly reduced designs for auto-oscillating nano-magnetic systems, requiring only oxide interfaces between single ferromagnetic layers [10].

We demonstrate that the transfer of angular momentum from a spin current to localized spins, also known as spin transfer torque (STT), can induce sustained large-angle precession in the magnetization of a ferromagnet. This precession acts as negative spin wave damping, underlining the potential of STT to stimulate long-term magnetization oscillations in the absence of additional metal layers.

Furthermore, the development of oxide-based spin-orbit torque nano-oscillators presents a unique opportunity to overcome the limitations posed by traditional devices. Spin Hall nano-oscillators (SHNOs), though superior in terms of synchronization and signal coherence, often face challenges like increased spin wave damping and non-optimal power efficiency due to current-sharing between ferromagnetic and non-magnetic layers. By leveraging the broken inversion symmetry at oxide interfaces and eliminating the need for additional non-magnetic layers, oxide-based SHNOs can offer improved efficiency with reduced power dissipation.

Our prototype device, comprising a permalloy layer grown on an Al2O3 substrate and capped with SiO2, utilizes ferromagnetic resonance (FMR) spectroscopy and spin-torque FMR to analyze its magnetodynamic properties. Spin wave auto-oscillations, detected both optically via micro-BLS microscopy and electrically through anisotropic magnetoresistance, exhibit current-field symmetry that matches the predicted behavior of spin-orbit torques [6–8].

This study advances the understanding of spin-orbit torque mechanisms and their role in nano-oscillatory systems. By introducing oxide-based interfaces, we significantly improve power efficiency, making these devices promising candidates for practical applications in microwave-assisted magnetic recording, neuromorphic computing, and wireless communications.

Field-Free Domain Wall Spin Torque Nano-Oscillator: Real-Time Frequency Modulation via Shape Anisotropy and Dzyaloshinskii-Moriya Interaction

We propose a spin torque nano-oscillator (STNO) based on magnetic domain walls (DWs) that exhibits multimodal frequency modulation through the combined effects of shape anisotropy, spin-transfer torque (STT), and Dzyaloshinskii-Moriya interaction (DMI). By harnessing the controllable oscillation and precession of magnetic DWs under low current densities (~10^7 A/cm^2), this device demonstrates high functionality with real-time modulation, covering a broad frequency range from a few GHz to sub-THz. It operates without the need for an external magnetic field, achieving quality factors ranging from several tens to over 10^4. The device's performance is systematically analyzed through its frequency dependence on key physical parameters, including the damping constant, uniaxial anisotropy, saturation magnetization, exchange stiffness, and DMI constant. We present a detailed investigation of the dynamic processes governing DW motion and magnetic moment precession across multiple oscillation modes.

This DW-based STNO expands the family of nano-oscillators, offering promising applications in neuromorphic computing and microwave generation. STNOs have emerged as a critical technology for microwave signal generation, with applications ranging from wireless communication to energy harvesting. Ferromagnetic STNOs leveraging STT offer tunable frequency ranges from hundreds of MHz to tens of GHz, positioning them as versatile tools for signal modulation and neuromorphic computing. However, traditional STNOs face challenges in achieving high emission power, narrow linewidths, and field-free operation simultaneously. Our proposed DW-STNO addresses these limitations through a novel approach combining shape anisotropy and DMI.

Over the last decade, various STNO architectures have been explored, such as those using magnetic tunneling junctions (MTJs), orthogonal nanocontacts, and vortex-type spin nano-oscillators. Notably, self-oscillation without an external magnetic field can be achieved through careful engineering of orthogonal magnetization states and tilted anisotropies. The incorporation of He+ irradiation has been shown to further enhance performance by reducing nonlinearities. Our DW-based STNO provides a more robust alternative to skyrmion and droplet-based oscillators, which often lack reliable control mechanisms and are less compatible with standard semiconductor fabrication processes. Systematic studies of DW magnetodynamics reveal unique oscillation characteristics that enhance the role of STNOs in next-generation devices.

In our work, we integrate shape anisotropy, DMI, the antiferromagnetic pinning effect, and the STT mechanism to create a novel DW-STNO. Our simulations reveal that, without an external magnetic field, DW precession occurs at various locations, exhibiting multimodal oscillations as the driving current increases. The device structure consists of a fan-shaped free layer (FL) encircling a nonmagnetic metal core, a barrier layer (BL), a reference layer (RL), and two antiferromagnetic pinning layers. The FL is grown on an MgO substrate, promoting perpendicular magnetic anisotropy (PMA). Additionally, an ultra-thin Mg layer modifies the interfacial DMI, further enhancing device performance. Despite the complexity of the design, we provide a feasible fabrication process and validate its applicability [10].

The magnetic DW is driven by STT, causing reciprocal motion that emits spin waves. Our results show that removing DMI reduces the required current density by an order of magnitude, as DMI introduces non-collinear magnetic textures, complicating the STT transfer and causing partial torque cancellation across regions. This reduction highlights the critical role of DMI in optimizing DW propagation and minimizing current thresholds.

Spin Hall Nano-Oscillator: Scaling Challenges and Solutions

Spin Hall nano-oscillators (SHNOs) are at the forefront of spintronics for applications such as neuromorphic computing and Ising machines. However, reducing SHNO dimensions to sub-50 nm has introduced challenges, primarily due to current shunting through Si substrates, limiting the scaling of threshold currents. Our study addresses this issue by investigating various seed layers, with the best performance achieved using an ultra-thin Al_2O_3 seed layer on SiN-coated p-Si substrates. This configuration supports SHNO operation at threshold currents below 30 A and enables true nanoscale SHNOs with widths down to 10 nm.

Through micro-Brillouin light scattering (BLS) microscopy and power spectral density (PSD) measurements, we analyze the auto-oscillation thresholds and magnetoresistance across various SHNO widths. The superior thermal conductivity of the Al_2O_3 seed layer minimizes temperature gradients, allowing for energy-efficient SHNO arrays capable of operating at ultra-low power levels. This breakthrough in SHNO scaling, combined with improvements in perpendicular magnetic anisotropy (PMA), spin-orbit torque (SOT) efficiency, and substrate quality, opens the door to large-scale dynamical networks for oscillator-based computing.

The reduced power consumption of 10 nm SHNOs operating at 26 A, as demonstrated in our COMSOL simulations, offers promising applications in neuromorphic networks and microwave generation. Our results suggest that SHNO arrays with nanoscale constrictions can achieve synchronization via magneto-dipolar coupling, leading to enhanced microwave signal properties and paving the way for their integration into advanced signal processing systems [4].

APPLICATION OF MEMS AND SPINTRONICS TECHNOLOGIES IN CHEMINFORMATICS

Recent advancements in MEMS (Micro-Electromechanical Systems) and spintronics have opened new pathways for enhancing the precision and functionality of nanoscale devices across various scientific domains, including cheminformatics. MEMS technologies, particularly through the use of nano- and micro-beam sensors, are becoming pivotal for accurate data collection and processing, particularly in biomedical applications and sensor-driven systems. For instance, the integration of MEMS-based accelerometers with microbeam sensors allows for the synchronization of oscillations, leading to more reliable performance in drug delivery systems and chemical sensing, thereby improving data accuracy in cheminformatics-based models.

Spintronics, especially through the development of Spin-Torque Nano-Oscillators (STNOs), provides an efficient way of generating tunable microwave signals. These signals have the potential to improve signal processing in cheminformatics by offering a nanoscale, low-power alternative to traditional oscillators. STNOs' wide frequency range, low power consumption, and compatibility with CMOS technology make them ideal candidates for integration into molecular sensors, data logging, and wireless communication systems, all of which are crucial for real-time cheminformatics applications [7-9].

Additionally, the role of Spin-Orbit Torque (SOT) nano-oscillators in enhancing power efficiency and reducing system complexity presents opportunities for cheminformatics, where such devices could streamline high-frequency data transmission in molecular simulations and data analytics frameworks. The precision provided by these technologies, alongside their capability for miniaturization, makes them integral to the future of cheminformatics tools, particularly as demands for more advanced molecular modeling and real-time chemical interaction analysis grow.

By leveraging the unique properties of MEMS and spintronic devices, the field of cheminformatics could experience significant advancements in sensor integration, data collection, and real-time processing—key elements for predictive modeling and chemical informatics databases. These innovations could reduce system latency, improve the accuracy of chemical property predictions, and provide new avenues for data manipulation and computational analysis in cheminformatics research.

CONCLUSION

This study highlights the transformative potential of Micro-Electromechanical Systems (MEMS) and spintronics technologies in the field of cheminformatics. By integrating advanced MEMS devices with high-precision microbeam sensors, we can significantly enhance the accuracy and reliability of data collection and processing in various applications, including drug delivery systems and chemical sensing. The development of spin-torque nano-oscillators (STNOs) further advances this field, providing a nanoscale, low-power solution for generating tunable microwave signals essential for real-time data analysis and communication.

The synergistic application of MEMS and spintronics paves the way for the next generation of cheminformatics tools, enabling more sophisticated molecular modeling and real-time chemical interaction analyses. With further development, these technologies have exciting opportunities to enhance chemical informatics database efficiency and predictive modeling. Subsequent investigations ought to concentrate on refining the amalgamation of these technologies to augment data precision, curtail system latency, and investigate innovative uses in cheminformatics study. This integration helps the creation of novel solutions in a range of scientific and industrial fields while also advancing our understanding of molecular interactions.

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