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How scanning probe microscopy can be supported by artificial intelligence and quantum computing?

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Abstract

The impact of Artificial Intelligence (AI) is rapidly expanding, revolutionizing both science and society. It is applied to practically all areas of life, science, and technology, including materials science, which continuously requires novel tools for effective materials characterization. One of the widely used techniques is scanning probe microscopy (SPM). SPM has fundamentally changed materials engineering, biology, and chemistry by providing tools for atomic-precision surface mapping. Despite its many advantages, it also has some drawbacks, such as long scanning times or the possibility of damaging soft-surface materials. In this paper, we focus on the potential for supporting SPM-based measurements, with an emphasis on the application of AI-based algorithms, especially Machine Learning-based algorithms, as well as quantum computing (QC). It has been found that AI can be helpful in automating experimental processes in routine operations, algorithmically searching for optimal sample regions, and elucidating structure–property relationships. Thus, it contributes to increasing the efficiency and accuracy of optical nanoscopy scanning probes. Moreover, the combination of AI-based algorithms and QC may have enormous potential to enhance the practical application of SPM. The limitations of the AI-QC-based approach were also discussed. Finally, we outline a research path for improving AI-QC-powered SPM.

Research Highlights

- Artificial intelligence and quantum computing as support for scanning probe microscopy.
- The analysis indicates a research gap in the field of scanning probe microscopy.
- The research aims to shed light into ai-qc-powered scanning probe microscopy.

KEYWORDS

artificial intelligence, automated experiments, machine learning, quantum computation, scanning probe microscopy

1 | INTRODUCTION

Scanning probe microscopy (SPM), including scanning tunneling microscopy (STM), atomic force microscopy (AFM), and scanning near field optical microscopy (SNOM) are universal tools for materials' surface characterization. Such scanning techniques enable the examination of the sample surface with even atomic resolution based on the measurements of the interaction between the probe tip and the sample surface (Bian et al., 2021). SPM enables to obtain a high-resolution 3D surface profile in a nondestructive measurement. It can examine samples of various types: metal, dielectric, semiconducting, biological, transparent, etc. without any special preparation (Lyu

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et al., 2023), usually in air or even liquid conditions, without vacuum requirement. Moreover, it is possible to combine SPM with different techniques to visualize several parameters simultaneously including electrostatic force (Sahare et al., 2023), electronic states (Ale Crivillero et al., 2023), ferroelectric domains (Huxter et al., 2023), electric potential (Iwaya et al., 2023), magnetic induction (Johnsen et al., 2003), adhesion (Hassani et al., 2021), hardness (Chen, Hu, et al., 2022a), stiffness (Petit et al., 2022), friction (Weymouth et al., 2022), topography (Cojocaru et al., 2022), chemical structure (Commodo et al., 2019), electronic structure (Yuan et al., 2020), electrochemical reactions (Asserghine et al., 2021), local stress (Haonan et al., 2022), impedance (Shkirskiy et al., 2020), resistance (Waldrip et al., 2020), electric current flow (Giridharagopal et al., 2019), thermal response (Vaziri et al., 2019), optical response (Lu et al., 2022), polarization (Baba et al., 2018), refraction index (Tranca et al., 2023), spin angular momentum of electromagnetic fields (Yin et al., 2020), fluorescence (Dey, 2022), photoluminescence (Soltanmohammadi et al., 2023), Raman (Mrđenović et al., 2023) and infrared spectra (Dopilka et al., 2023). Besides its measuring capabilities, SPM can be used to create and modify the structure. It can be done in several ways. First, the simplest techniques rely on mechanically carving patterns in soft material with the use of the AFM probe (Pellegrino et al., 2022). The second possibility is to precisely illuminate a photoresist layer through the SNOM probe to create a mask for photolithography (Aghaei et al., 2015; Roszkiewicz et al., 2019). Another technique, called dip-pen nanolithography, uses the probe to absorb the "ink" molecules and release them on the surface during contact mode (Liu et al., 2019). Thermal scanning probe lithography is used to directly melt or ablate the substrate (Howell et al., 2020). Another technique, field-emission scanning probe lithography, utilizes an electron field emission from the probe material, when a high voltage is applied to the probe (Behzadirad et al., 2020). Besides nanolithography, SPM is also a nanomanipulation tool that allows precise building of desired structures by fine manipulation of small objects (nanoparticles, nanotubes) with the probe tip (Park et al., 2017).

SPM faces also some serious challenges (described in more detail in Section 4) connected, among others, with contamination or destruction of the probe or sample during scanning, inaccurate surface mapping due to local defects, tip-sample convolution, slope tilt or overhangs, suboptimal feedback setup, far-field noise, thermal drift, piezoelectric hysteresis, scanner creep, calibration errors. Optical techniques combined with AFM are additionally the source of troublesome optical and chemical artifacts.

Efficient and fast analysis of samples obtained by application of scanning probe microscopy remains a challenge, especially for samples with high attenuation or non-trivial geometries. To understand the spectrum of a sample obtained using SNOM, it is also necessary to specify a wide range of experimental variables such as illumination angle and frequency, the geometry of the tip, and its tapping amplitude. The Artificial Intelligence (AI)-based approach, which already has a wide field of applications, including wastewater treatment (Malviya & Jaspal, 2021; Zhao et al., 2020), circular economy (Pregowska et al., 2022), agriculture (Zhang et al., 2021), adsorption studies (Mahmoodi et al., 2018; Tanzifi et al., 2017), graphene and graphene-based materials characterization (Huang et al., 2022), mechanical studies of carbon nanotube-based nanocomposite (Ho et al., 2022), magnetic hyperthermia (Osial & Pregowska, 2022), optimization of materials properties in cancer diagnosis and treatment (Govindan et al., 2023), early diagnosis of polycystic ovaries syndrome (PCOS) (Nsugbe, 2023), cancer research (Elemento et al., 2021), opened new possibilities in the scanning probe microscopy field (Chen, Xu, et al., 2022b). Since AI provides fast extraction of information contained in image data, thus, the application of statistical tools and AI-based algorithms can significantly increase the efficiency and productivity of microscopy, for example, image processing and pattern recognition in scanning transmission electron microscopy (STEM) (Konečná et al., 2022; Ziatdinov et al., 2020), or enhanced data acquisition and analysis in scanning probe microscopy (Fan et al., 2022). AI can be applied to recognition and assigning identities on images, while it enables the detection of specific molecules in complex biological processes enhancing or even replacing hand-engineered features. It is helpful in image segmentation, where the task is to identify whether each pixel belongs to a structure category.

Over the past 70 years, digital computers have made significant progress, from mastering the game of chess to solving complex algebra problems at the school level. The initial enthusiasm for AI peaked with optimistic discussions about household robots that make housework easier and even serve as babysitters. But as media coverage intensified, so did the shadow of skepticism. During these challenges, a promising path has emerged–the convergence of AI and quantum computing (QC) (Krenn et al., 2023). AI, with its ability to learn complicated tasks, combined with the computing power of quantum computers, offers a unique opportunity for groundbreaking research. This synergy has opened new doors, especially in the processing of huge amounts of data generated during the characterization of nanomaterials using SPM microscopes (Chen et al., 2023). The integration of AI and quantum computers allows us to construct learning machines that can distinguish certain properties, such as crystal and electronic structures, from existing electronic data related to nanomaterials. This advancement allows AI to provide valuable insights into potential plasmonic and metamaterial properties, as well as the conditions under which they are generated. As we embark on this exciting journey at the intersection of AI and quantum computing, the possibilities to advance research and overcome previous limitations seem limitless. We are very optimistic about further progress and the transformative impact that this collaboration can bring. The potential possibilities mentioned above are discussed in the following part of this article, using the example of sophisticated SPM microscopes and the digital data generated with their help. The paper is organized as follows: Section 2 describes materials and methods, Section 3 presents the principle of scanning probe microscopy, Section 4 lists the challenges faced by SPM, Section 5 presents the theoretical and numerical modeling applied in SPM, Section 6 presents next-generation scanning probe microscopy powered by AI, Section 7 contains the challenges encountered in SPM supported by AI and QC, Section 8 lists the limitations of using AI in

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SPM, while Section 9 contains the discussion and conclusions, and Section 10 presents some future remarks.

2 | RESEARCH METHODS

We employed a systematic review approach adhering to the PRISMA Statement (Liberati et al., 2009) and its extension, PRISMA-S (Rethlefsen et al., 2021) to systematically evaluate recent publications, reports, protocols, and review papers retrieved from Scopus and Web of Science databases. The data retrieval process involved both electronic and manual searches. The research commenced with a search for relevant research articles to include in the study. The used keywords were: scanning probe microscopy, scanning near-field optical microscopy, scanning tunneling microscopy, atomic force microscope, quantum computing, Artificial Intelligence, Machine Learning, Artificial Neural Networks, and their variations. Based on the research questions:

> **RQ1.** How Artificial Intelligence and data-driven approaches can improve scanning probe microscopy?

> **RQ2.** If convergence of AI and QC has the potential to increase the efficiency of SNOM?

The scope of the study was established, specifying the search period, publication quality, and publication types. Additionally, the chosen sources were scrutinized for alignment with the research topic, and their contribution to nano-spectroscopy was evaluated. Selected texts have been given a certain level of confidence in quality (Gough et al., 2017). The search focused on English-language full-text articles, including electronic publications prior to print. Exclusion criteria included doctoral dissertations and materials not related to SPM and AI/ML. After retrieving and analyzing the relevant articles, a total of 263 documents were included in the analysis. The main limitation of the presented study was the fact that in the case of experimental data, only selected data are demonstrated in the literature, and limited access to the data is gained, which can affect the output data. What is more, many different materials are investigated with different techniques, where not only experimental factors should be included as the input but also the type of tools including technical issues. Another issue is the reproducibility of the obtained results, inaccuracy and unreliable selection of input data, incomplete data, and/or complexity in the data.

3 | SCANNING PROBE MICROSCOPY—WORKING PRINCIPLE

Scanning probe microscopy is a measurement technique, which allows materials characterization at the atomic level, in particular exploring the local properties of a sample surface with high resolution. It was established in 1982 when Swiss scientists presented the scanning tunneling microscope to investigate a surface with a spatial resolution at the atomic level (Binnig et al., 1982). This approach is based on the quantum tunneling phenomenon, where a bias voltage is introduced between the surface and a tip, separated by a 0.4–0.7 nm distance in a vacuum. As a result, electrons tunnel through the gap between the tip and the sample, and this tunneling current is a function of the applied voltage and the local electronic density of the states of the sample. The next big step in the history of microscopic measurements was the discovery of the optical near-field scanning microscope (Lewis et al., 1984; Pohl et al., 1984). Its operating principle is based on the treatment of the light scattered from a very small gold nanoparticle as a new light source, that is, utilizing a propagating far field (Synge, 2009). The excitation and detection of diffraction in the near field are used as microscopic imaging tools, during which the scanning process takes place. According to the Rayleigh criterion, two light lines can be distinguished if the maximum of one diffraction pattern coincides with the minimum of the second one. The resolution of standard light microscopy is limited by the wavelength of light. Subsequent corrections led to achieving a resolution of about 180–200 nm (with the use of immersion oils). SNOM, on the other hand, uses an evanescent near field that carries high-resolution spatial information, but its intensity decreases exponentially with increasing distance from the source. As a consequence, SNOM resolution is limited by the aperture dimensions and probe-sample distance and can be lowered to about 50 nm. Table 1 and Figure 1 summarize the most important milestones in the evolution of scanning probe microscopy.

SPM is applied to examine surfaces with atomic-scale resolution. During measurements, a sharp probe is scanned over a sample surface to collect local information concerning the properties of examined materials. The typical separation between the tip and the sample is about 0.1–10 nm. The forces arising between the tip and surface are utilized as a feedback mechanism to regulate the probe-sample distance and bending of the cantilever. The distance and motion of the probe can be controlled through tunneling current assessment, optical deflection control process, fiber interferometry, or piezoresistive techniques (Seo & Jhe, 2007) The forces that appear between the probe apex and the surface can be classified as attractive, including van der Waals interactions, electrostatic interactions, chemical (covalent bond) interactions and capillary forces (in the presence of a liquid film); or repulsive, including Coulomb interactions between electrons, hard-sphere repulsion (Hertzian contact), and Pauli exclusion repulsion (Ishida & Craig, 2019). Each of those interactions is characterized by a different range and strength and their relative influence depends on the tip-sample interval. It is worth noting that the repulsive forces, in general, have a very slight range with inverse power law or exponential decaying dependence of the distance. The resultant complexity of force interaction can make the interpretation of obtained images difficult and ambiguous (Bowen & Hilal, 2009).

The operating modes of the SPM depend on the type of microscope and application. There are four basic modes: contact mode (Zhang et al., 2020) (the tip is constantly in contact with the surface during scanning), tapping mode (Dos Santos et al., 2022) (the tip vibrates at its resonant frequency or slightly below, gently tapping the

TABLE 1 The crucial milestones in scanning probe microscopy.

Year	Milestone	The quintessence of discovery	References
1982	Scanning tunneling microscope	The bias voltage introduced between the tip and sample surface facilitates electron tunneling across the vacuum gap. Resolution: 0.1 nm (horizontal), 0.01 nm (vertical).	(Binnig et al., 1982)
1984	Optical near-field scanning microscope	Exploits an evanescent near-field extending beyond the aperture of diameter < λ. Optical resolution is limited by the aperture diameter.	(Lewis et al., 1984; Pohl et al., 1984)
1985	Scanning capacitance microscope	A capacitor is formed between a sharp conducting probe and a semiconductor sample. A bias introduced between the tip and surface of the sample generates capacitance variations.	(Matey & Blanc, 1985)
1986	Atomic force microscope	Measures of forces between the mechanical probe and sample. Piezoelectric elements precisely control the movements of the tip. The resolution is even below 1 nm.	(Binnig et al., 1986)
1986	Scanning thermal microscope	Maps the local temperature and thermal conductivity of an interface with thermal probes (thermocouple, resistive, or bolometer probes).	(Williams & Wickramasinghe, 1986)
1987	Magnetic force microscope	Utilizes a sharp magnetized tip to probe the magnetic landscape of a sample, enabling the visualization of distinct magnetic domains, including Bloch and Néel walls, closure domains, recorded magnetic bits, and the dynamic behavior of domain walls under the influence of an external magnetic field.	(Martin & Wickramasinghe, 1987)
1987	Inelastic electron tunneling spectroscopy	Possibility to obtain well-defined vibrational spectra from different parts of the same molecule with the STM probe operating in liquid helium.	(Smith et al., 1987)
1988	Electric force microscope	EFM consists of a tip vibrating near a surface and an optical heterodyne detection system to precisely measure its vibrations. Possibility to evaluate tip displacements spanning significant distances and a broad spectrum of frequencies.	(Martin et al., 1988)
1988	Inverse photoemission microscope	Detection of light emitted as a result of the inverse photoelectric effect of electrons introduced at a surface through tunneling from a probe. Provides detailed spectroscopic data on the density of unoccupied states and local resonances with an almost atomic resolution across a spectrum of photon energies. Possibility of spatial mapping of optical transitions.	(Coombs et al., 1988)
1989	Scanning electrochemical microscope	A miniaturized electrode scans over a submerged sample to capture current fluctuations, which are determined by the surface morphology and electrochemical activity of the sample. Possibility to quantify material transfer from a surface with exceptional spatial and temporal precision.	(Hüsser et al., 1989)
1989	Scanning ion-conductance microscope	The tip is an electrode. The non-conducting samples are immersed in aqueous media conducting electrolytes. Measurement of the increase of access resistance in a micropipette when it approaches the surface.	(Hansma et al., 1989)
1989	Scanning spin-precession microscope	The electron spin precession in a magnetic field generates a fluctuation in the tunneling current, resonating at the Larmor frequency. This radio-frequency signal is confined to regions less than 1 nm in size. Possibility to detect and distinguish individual paramagnetic atoms, spins, and surface defects.	(Manassen et al., 1989)
1990	Photovoltage scanning tunneling microscope	Photoexcited carriers are drawn towards and accumulate at local potential minima on the surface, leading to enhanced photovoltage. Possibility to investigate both surface and bulk properties, including bandgap variations, doping density changes, and strain field variations.	(Hamers & Markert, 1990)
1990	Photon scanning tunneling microscope	The topography of the sample perturbs the surface wave. Photons tunnel between the surface and the probe allowing to measure changes in the evanescent field. No necessity for an electrically conductive surface.	(Reddick et al., 1990)
1991	Scanning chemical potential microscope	By monitoring the electrical current and thermoelectric voltage generated at the tip-sample junction, this technique offers a direct and sensitive method for assessing atomic-level variations in the surface chemical potential gradient of the heated sample.	(Williams & Wickramasinghe, 1991)
1991	Kelvin probe force microscope	Measurements of the surface work function contain information about the local composition and electronic state of the surface. The work function is connected to atomic composition, surface defects, catalytic activity, corrosion, trapping of charge in dielectrics, doping and bending of semiconductor bands, phase state, and force distribution on surface reconstruction.	(Nonnenmacher et al., 1991)
1994	Apertureless near-field optical microscope	Detecting the modulation in the electric field of the wave scattered from the sharp tip scanned in immediate contact with the sample surface. Increased resolution of SNOM to the nanometer regime.	(Zenhausern et al., 1994)

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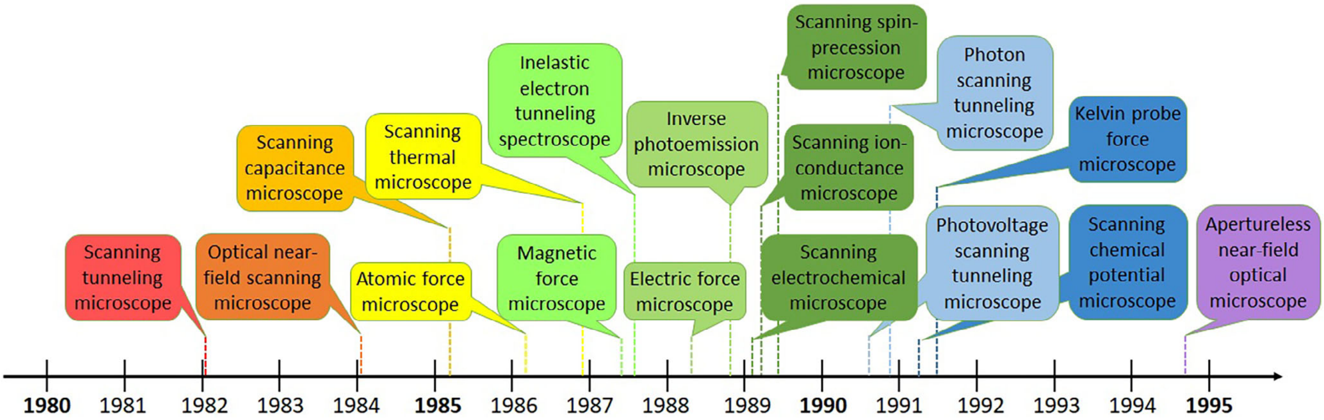

FIGURE 1 The most important milestones in the development of SPM (Binnig et al., 1982; Pohl et al., 1984; Lewis et al., 1984; Matey & Blanc, 1985; Binnig et al., 1986; Williams & Wickramasinghe, 1986; Martin & Wickramasinghe, 1987; Smith et al., 1987; Martin et al., 1988; Coombs et al., 1988; Hüsser et al., 1989; Hansma et al., 1989; Manassen et al., 1989; Hamers & Markert, 1990; Reddick et al., 1990; Williams & Wickramasinghe, 1991; Nonnenmacher et al., 1991; Zenhausern et al., 1994).

sample), non-contact mode (Freund et al., 2018) (the tip vibrates slightly above its resonant frequency above the surface without touching it) and shear force mode (the cantilever oscillates parallel to the surface) (Quacquarelli et al., 2015). In addition, the constant mode can be performed under the mechanism of preserving constant force or constant height between the tip and the surface. The real-time feedback system allows controlling the tip-sample distance with high accuracy that could reach even ~0.01 Å. In fact, the extensions of the original SPM allowing the gathering of various information about the sample initialized a rapid growth in the field. In combination with the possibility to examine different sample types (metal, semiconductor or dielectric, transparent or opaque) SPM can find its applications in many branches of nanotechnology (Barron et al., 2022) (nanophotonics, nano-optics, nanolithography), physics (Lindner et al., 2020), chemistry (Gusenbauer et al., 2019), two-dimensional (2D) materials research (Firestein et al., 2020), epitaxial thin-film (Lavini et al., 2020) and electronic circuit components (Moreno-Moreno et al., 2019), biology (Pandey et al., 2021), climate (Madawala et al., 2021), food (Liu & Yang, 2019), pharmacy (Piergies et al., 2018), criminalistics (Cavalcanti & Silva, 2019), to name a few.

4 | SCANNING PROBE MICROSCOPY—CHALLENGES

Despite its various advantages, SPM also has some disadvantages. A serious limitation is the fact that the information is obtained only from a surface, which automatically excludes a deeper, volume analysis (Summerfield et al., 2019). Another downside is the very small operating tip-sample distance, while the high-resolution images require a long scanning time (Elemans, 2016). Thus, the limited vertical range of a probe restricts the allowed roughness of the examined surface (Zubar et al., 2020). Another drawback is that the probe is scanned slowly over the surface, resulting in extended scanning time, which may introduce thermal drift in the image. Consequently, this might pose challenges when measuring precise distances between topographical features in the image (Kim et al., 2022). As a consequence, a relatively small single scan image size (i.e., maximal about 150×150 μm) is achieved. Another issue is connected with the measurements of the soft materials. Such surfaces examined in a contact or shear force mode might be dragged by the tip or stuck to it, falsifying the outcome (Pinto et al., 2020). On the other hand, hard materials may damage the probe and thus significantly lower the image quality and lifetime of the probes (Shi et al., 2020).

Interpretation of the images acquired from SPM requires a detailed analysis of the tip-sample interactions. Optimization of the SPM operation can be very laborious and subject to operator error in terms of sample specifications as well as personal experience (Bian et al., 2021). The multiple types of artifacts can blur the final data and raise doubts about the correctness of the results. The sources of the artifacts in AFM can be various, for example: contamination or damage of the sample, damaged, blunt, or contaminated probe tip which may distort the resulting image (Voigtländer, 2019), local defects, tip-sample convolution, slope tilt or overhangs, suboptimal feedback setup, far-field noise, thermal drift, piezoelectric hysteresis, scanner creep, calibration errors. In the case of AFM-based imaging of the biological samples, the generation of lateral forces may contribute to the movement of the sample, or even to its destruction (Muzyka et al., 2023). Moreover, cantilever amplitude during biological sample measurement is sensitive to the sample's structural, mechanical, and chemical properties, leading to potential interference with the accuracy of the measurement (Sumbul & Rico, 2019). AFM is also inaccurate in the case of measurements of several-layer graphene (Wang, Jia, et al., 2023a). The number of possible artifacts increases when AFM is combined with other microscopy techniques like SNOM. The artifacts arising from SNOM are connected with far-field disturbances, shifts between the optical signal and topography, optical contrast (for example interference pattern, artificial stripes, contrast inversion,

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phase change), or chemical contrast (absorbance, fluorescence, Rayleigh scattering, Raman scattering, polarization, unknown specific shear-force responses), etc. An additional concern arises from the drawbacks of fluorescent probes and slide preparations that involve fluorescent cells. Only in extremely thin samples, these methods do not introduce blurring into the measurements because the fluorescent signals originating beyond the depth of field of the lens are eliminated (Sanderson, 2023). All those artifacts may lead to images that significantly differ from an actual surface (Hecht et al., 1997; Nörenberg et al., 2021; Sheremet et al., 2019).

5 | THE THEORETICAL AND NUMERICAL MODELING IN THE SCANNING PROBE MICROSCOPY

To conduct experiments more effectively, it is crucial to model the process, including the application of Finite-Element Methods (FEM) (Kindt et al., 2004; Liu et al., 2004). For example, the tip geometry in SNOM can be modeled using FEM (Sychugov et al., 2008). It turned out that by modeling the interaction of tip geometry and protective metal coating it is possible to refine the experiment before selecting the desired tip configuration. Thus, the tip can be assumed in simple models as a perfect sphere (Becerril et al., 2023). The more complicated FEM model of SNOM-tip was proposed in Reference Hafner et al. (2017). It accounted for the presence of a scatterer in the frequency domain in the form of data-sparse non-local surface-impedance boundary conditions. To reduce computation time the conversion of a sparse finite element (FE) matrix to $\varkappa$-matrix and approximation by adaptive cross approximation algorithm (ACA) to construct the $\varkappa$-matrix have been applied. Numerical methods are also useful when designing apertureless SNOM probes modified with metal or dielectric indentations in order to achieve local near-field enhancement at the apex of the probe (Qian et al., 2015). The occurring local geometric resonance, the standing wave resonance of surface plasmon polariton, and the Fano resonance are modeled with the FDTD method. FEM-based methods can be also applied to the modeling of mechanisms for creating nanopatterns on noble metal nanolayers (Wang, Cui, et al., 2023b). It was suggested that the main factor to consider when modeling is the melting and transformation of the nanofilm under the tip. FEM can be also applied to the calculation of the real-space electromagnetic field (Guo, Li, et al., 2023b; Guo, Wu, et al., 2023a; Hu et al., 2023; Lu et al., 2023). In Reference Granchi et al. (2023), artificially created FEM maps were compared to the experimentally inferred spectral shift maps to evaluate the distribution of electric field strength. The optical quality factors as a function of the structural parameters (wall thickness and central hole radius) were calculated from the non-Hermitian perturbation theory (Lalanne et al., 2018) These maps can also be obtained by evaluating the total radiating dipole moment of the tip (Fei et al., 2012; Luan et al., 2023). On the other hand, in the case of AFM measurement FEM-based computation can be used to determine the material loss and surface finish (Jain et al., 1999) or reproduce the microscopic deformation process (Liang et al., 1999). The development of FEM-based methods was proposed in Reference Xue et al. (2023), namely the application of the coupled mechanical–electrical finite element approach to the prediction of the reaction of piezoelectric materials to external stimuli. Another approach is the modeling of the material structure and vibrational spectra with the Density Functional Theory (DFT) to evaluate the interaction at the molecular level (Primera-Pedrozo et al., 2023). DFT can be treated as a complement of experimentally obtained spectra (Grudinin et al., 2023; Schirmer et al., 2023). Thus, the combination of FEM and DFT has the potential to expand the understanding of nanomaterials' structures and their optimization, including surface (Xiong et al., 2023). For example, in Reference Xing et al. (2023) these techniques were combined in the field of scanning Kelvin probe force microscopy analyses of the influence of crystal structure on hydrogen diffusion in α-Fe and γ-Fe.

The modeling of the tip interaction also makes it possible to improve the microscope calibration process, which can be quite long. It can be done in two ways. The first one is computationally expensive and complex, while it requires an approximation of the system of the probe and the sample to an invertible model (Govyadinov et al., 2014). The second one is black box calibration models. This approach enables the extraction of the permittivity without detailed electromagnetic interaction modeling. However, the black box method is designed for stationary systems, and the distance between the probe and the surface is slowly modulated, for example in the case of s-SNOM (Guo, He, et al., 2023c; Hillenbrand et al., 2001). In Reference Siebenkotten et al. (2023), calibration method that takes probe tapping into account in extracting the time-invariant sample permittivity was shown. It is based on fitting the Drude model for free electrons to the measured permittivity in the infrared spectral range. In Reference Grudinin et al. (2023), the quantitative s-SNOM model approximates the tip as an elongated conducting spheroid and computes signals from the total radiating dipole moment of the tip. On this basis, parameters such as the Drude weight and electron scattering rate of graphene-supporting propagative plasmons can be obtained.

The numerical methods are also implemented to model physical phenomena that occur during scanning, giving a contribution to the understanding of the experimental data. In Reference Azib et al. (2018), the AC–DC module of COMSOL Multiphysics® was used for modeling an electrostatic force-distance curve (EFDC) between an AFM tip and an electrically charged electrode embedded within a thin insulating layer. The study found that the tip and cantilever contributions to the lateral and vertical potential distribution are significant and must be considered during the interpretation of EFDC measurements. Numerical calculations were also used to explain the underlying mechanisms that contribute to the degradation of asphalt concrete due to moisture at the asphalt-aggregate nanostructured interfaces (Dong et al., 2017). The PeakForce Quantitative Nanomechanics AFM was assisted with the Molecular Dynamic simulation (Materials Studio 6.0, Accelrys) based on Lennard-Jone's potential. The calculations revealed the complex structure of the asphalt-aggregate interface and its weak points in the form of

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water-dissolving asphaltenes and polar aromatics that lead to interface failure. Analytical (Argatov et al., 2023) and numerical (Valero et al., 2016) models are also used to determine the mechanical properties of soft biological samples that can be characterized only through nanoindentation tests with the use of an AFM tip. The numerical simulations also allow us to determine the reasons for the increased contamination of fluids sterilized by microfiltration when bacteria are treated with sub-lethal concentrations of antibiotics (Gaveau et al., 2017). The AFM nanoindentation measurements revealed that antibiotics reduce the elasticity of bacterial cell membranes and make the walls of bacteria more susceptible to deformation, which leads to increased migration of cells through porous membranes.

6 | NEXT-GENERATION SCANNING PROBE MICROSCOPY POWERED BY ARTIFICIAL INTELLIGENCE AND QUANTUM COMPUTING

Since AI, including Machine Learning (ML) enables efficient analysis of a huge amount of data, it can be considered a powerful computational tool to solve complex problems related to pattern recognition, function estimation, and classification problems (Liu, Kelley, Vasudevan, Funakubo, Ziatdinov, & Kalinin, 2022a). AI techniques also enable inferences about structures that would be difficult to model (Liu, Morozovska, Eliseev, Kelley, et al., 2023a). Recently, in image processing the deep learning-based approach, that is, neural networks with a number of hidden layers, has become the dominant methodology in the field of medical image recognition, segmentation (Dietler et al., 2020), and classification (Gao et al., 2019). This type of network, based on the input data being a photo or a photo-like image, performs classification and regression tasks. The advantage of deep learning is that it can search the parameter space for the best match of the target and get a solution after the learning phase, in contrast to optimization-based approaches. In the case of scanning probe microscopy, AI-based algorithms can be applied to minimize the need for human action during measurements, and even partially eliminate it (Vasudevan et al., 2021). Thus, the automatization of the measurement processes should not be used to eliminate human participation, that is, autonomous experiment (AE), but since the microscopy experiments are well-defined when we take into account prior physical knowledge, rather than automate routine operations (Kalinin et al., 2021). The schematic idea of the AI/ML-based application in SPM is shown in Figure 2.

In a deep neural network (DNN) that consists of three layers: an input, an output layer, and at least one hidden layer, artificial neurons are connected with the weight, whose values are selected in the learning process (LeCun et al., 2015). Hidden layers provide the nonlinear mapping between input and output layers. The effectiveness of these approaches leads to the choice of input data (number and quality), the number of hidden layers, the choice of lost function, the learning rate, and initial weights (Goodfellow et al., 2016). DNN can be applied in retrieving subwavelength dimensions based on exclusively far-field data to predict the geometries of the nanostructure, mainly the system of bidirectional network, in which the first one is a geometry-predicting-network (GPN), while the second Spectrum-predicting-network (SPN) (Malkiel et al., 2018). In fact, this is an application of DNNs to solve the inverse problem (Yao et al., 2019). A similar approach can be found in the designing of metasurfaces (Liu et al., 2018), where the inverse problem was formulated as deriving the dielectric function of materials exhibiting subtle or pronounced resonances from experimentally acquired near-field spectra using feed-forward neural networks (FFNNs) proposed. Also,

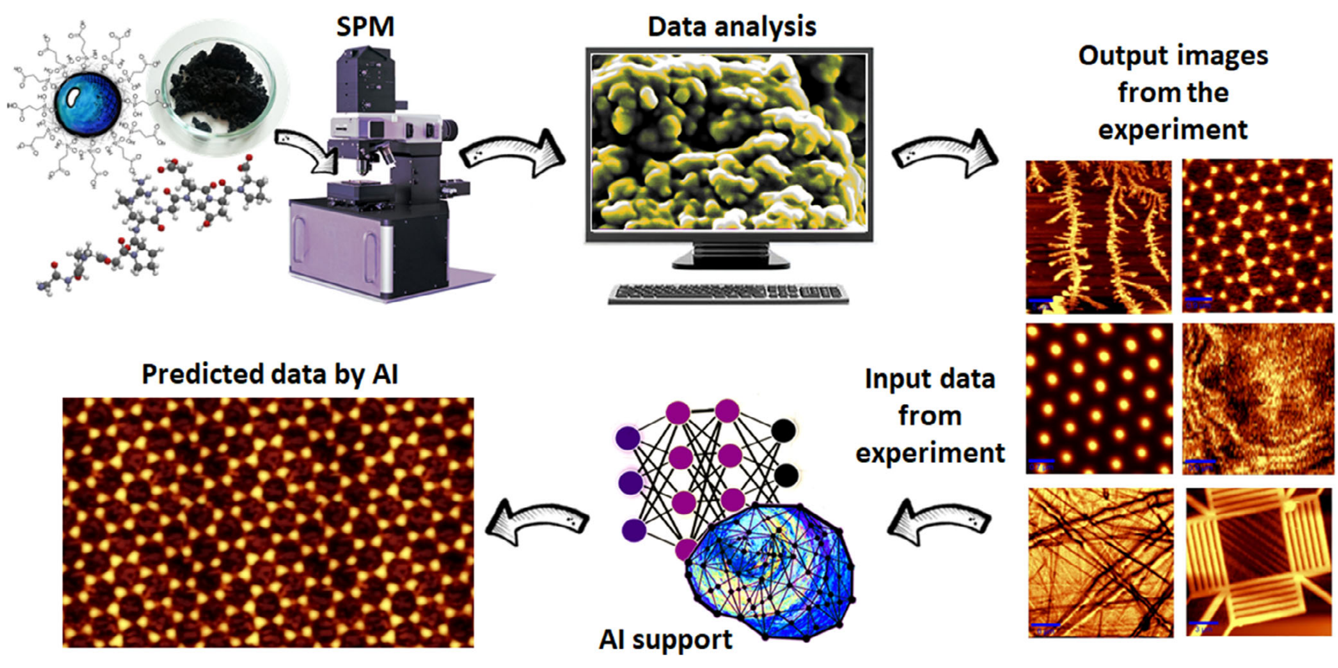

FIGURE 2 Schematic illustration of AI use in SPM analysis.

DNN was proposed to retrieve the parameters of a physical object from its scattering pattern with the resolution wavelength/10 (Pu et al., 2020). The proposed network architecture consists of four fully connected layers activated with ReLU function and three neurons. The learning algorithm was Adam's stochastic optimization method and the mean absolute error loss function. AI-based solutions can also be applied to the reduction or complete elimination of the time-consuming routine procedures in scanning probe microscopy (Huang et al., 2018), like, for example, the autonomous SPM operation platform (DeepSPM), which is based on CNNs (Krull et al., 2000). It enables assessment of the quality of the acquired images and the condition of the probe.

Thus, the most popular deep learning algorithm used for image processing is the convolutional neural network (CNN) (Alldritt et al., 2020). They contain fewer connections than standard networks with a similar number of hidden values, which makes them easier to train without significantly losing accuracy. This is possible thanks to the operation that allows the flow of information in many planes, that is, a filter or kernel consisting of a small array of weights (Krizhevsky et al., 2012). This is beneficial for image analysis. Using the CNNs advantage, which allows the ignoring of irrelevant features in the analysis, such as signal and noise in the ground area, SNOM images can be effectively analyzed (Azuri et al., 2021). On a millisecond timescale, convolutional neural networks (CNNs) can effectively extract the wavelengths and quality factors of polariton waves from images (Duan et al., 2021). In addition, CNNs outperform traditional Fourier transforms in extracting multiple wavelengths for hyperbolic waveguide modes (Xu et al., 2021). A 1D supervised CNN can work as a fully automatic technique generating chemical concentration maps from hyperspectral images obtained with Stimulated Raman Scattering (Mozaffari et al., 2022). This approach can also be used for the dispersion of quasiparticles (Cao et al., 2018), evaluation of twist angles, Fermi level lattice parameters, or electron localization degree with Moiré super-lattice imaging (Peng et al., 2023). Thus, achieving high CNN accuracy heavily relies on the optimal selection of hire parameters, which is related to the need to provide a large amount of high-quality data (Chen et al., 2021). In Reference Rashidi and Wolkow (2018), a CNN was employed to assess the SPM tip quality by analyzing images of known atomic defects on a hydrogen-terminated Si(100) substrate. The proposed network architecture comprises two convolutional layers, one pooling layer, one densely connected layer, and one output layer. It enables automatic identification and isolation subsection of an image obtained using STM. The inputs to the network are fragments containing dangling bonds. On their basis, the network evaluates the quality of the tip. Also, the algorithms based on K nearest neighbor (KNN), Random Forest (RF), Support Vector Machine (SVM), and fully connected neural network (FCNN) with 18 hidden layers with rectified-linear-unit (ReLU) activation function and Adam optimizer was applied for this purpose (Kingma & Ba, 2014). The results obtained can be used to develop autonomous atomic-scale production tools. The CNN has been also proposed to be an unattended SPM data acquisition system, namely system DeepSPM (Krull et al., 2000). The network is based on 12 convolutional layers and 2 fully connected layers. It was trained with the Adam optimizer (Kingma & Ba, 2014) with a cross-entropy loss. The system operates as a control loop, scans the sample, and accepts only samples classified as good for analysis. If the sample is classified as bad, it looks for causes such as loss of sample-probe contact, probe failure, error sample region, and invalid probe. In turn, Auto-CO-AFM is an open-source package based on CNNs, which enables the evaluation of the tip functionalization procedures (Alldritt et al., 2022).

Another application of neural networks as a classification tool was shown in Reference Burzawa et al. (2019). The feed-forward neural network was applied to surface classification based on spin configurations in the case of strongly correlated electronics systems. When the images are near criticality, the spin configuration was obtained with the application of a theoretical mode (Carlson et al., 2015). The various algorithms can also be combined to provide higher accuracy, like in Reference Menaka and Vaidyanathan (2023), where the CNN was combined with SVM to differentiate chromosomes into 24 classes. In the first step, to increase the resolution of the input data, the input data was converted using super-resolution models, in particular, the Laplacian pyramid super-resolution network (LapSRN) (Lai et al., 2019). Next, the SVM was used to label the input data, and CNN, which consists of six convolution layers, and three pooling layers was applied as a classifier. To increase the accuracy of the network, the Swish activation function was used instead of the ReLU activation function. The intensity profiles perpendicular to the edges, as well as the corresponding edge positions, were the input data to CNN to enhance the microscopic image resolution (Tsai & Yeh, 2021). Another interesting solution, namely the open-source classification tool for crystalline 2D phases in AFM images (Automated identification of Surface images—AiSurf) was proposed in Reference Corrias et al. (2023). It enables the detection of automatically performed analyses such as detecting the distribution of interatomic vectors and deviations from ideal lattices. Also, the use of unsupervised independent component analysis based on non-Gaussianity and statistical independence of data to the Raman spectra of mixtures allows one to extract individual component signals and differentiate organelles in cells by their biochemical compositions without any external labels (Mozaffari & Tay, 2022).

On the other hand, in Reference Ziatdinov et al. (2022), an attempt to reproduce the decision-making process of the person experimenting, namely piezoresponse force microscopy analysis of phase transitions induced by the varied concentrations of Sm dopant in BiFeO3, is shown. This approach combines Gaussian process-based active learning (GP-AL) and Bayesian optimization (GP-BO) procedures. In Reference Chi et al. (2022), an indirect adaptive iterative learning control (iAILC) scheme based on iterative dynamic linearization is shown to improve the P-type controller correction response. Learning from setpoint gain is controlled by an adaptive mechanism in real-time. As a result, a linear data model for algorithm design and performance analysis can be obtained for the strongly nonlinear and nonaffine structure of the systems.

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AI is also a powerful tool in various types of disease diagnosis. Thus combining AI-based algorithms with SNOM can be useful in the accurate determination of even biological samples, including cancer cells. In Reference Ellis et al. (2021), multivariate metrics analysis (MA) technique was applied to the precise determination of the system of oral squamous cell carcinoma (OSCC) nodal metastases embedded in the lymphoid tissue with the IR-SNOM (Fourier transform infrared spectroscopy combined with SNOM). The MA-based algorithm can discriminate between two different tissues based on the highest-ranking metric, and as a consequence, provides the possibility of analysis of the chemistry of tissues. In Reference Ciasca et al. (2019), FFNNs were applied to the medical diagnostics of Glioblastoma multiforme (GBM). The summary of different AI-based models and their applications in SPM are presented in Figure 3.

An important problem in data analysis is the analysis of noisy data. Here, AI-based approaches are very helpful. This operation can be carried out in many ways, one of them is presented in Reference Borodinov et al. (2019) the application of the deep neural network, which was combined with the least-square approach to extract specific parameters from multidimensional data obtained with the use of spectral-imaging techniques combined with scanning probe (also electron and optical) microscopy. This allows for examination of a wide range of materials for which the excitation is low, and also possibly reduces the need to average signal in time. This approach improves the signal-to-noise ratio of noisy data and enhances pattern recognition, which allows for extracting various material properties from weaker signals.

AI, besides many unquestionable advantages, has some inherent drawbacks. A significant limitation in the development of accurate algorithms is too little data to train them and/or data of poor quality (Barnard et al., 2019). Thus, data management procedures, in particular, the standards of data annotations with a special emphasis on the Findable, Accessible, Interoperable, Reusable (FAIR) guiding principle are fundamental and are of high importance (Rodani et al., 2023; Wilkinson et al., 2016). In the area of AI, there are two approaches, the first is to work on theoretical (simulated) data like MoleculeNet (Wu et al., 2018) and the second is the use of experimental measurements like, for example the place to store, share, and search in the form of public database SPMImages (SPM Portal, n.d.). An interesting public database was created with the application of Artificial Intelligence, in particular CNN, namely density functional theory (DFT) STM for two-dimensional (2D) materials (JARVIS, n.d.; Choudhary et al., 2021). It contains data for 716 exfoliated 2D materials, calculated using the Tersoff-Hamann method. Also, by supporting FEM methods, the training and test data sets can be extended with artificially generated data, and as a consequence more efficient algorithms can be developed.

On the other hand, the AI-based algorithm and quantum computation have a huge potential to complement each other and stimulate mutual development (Zhu & Yu, 2023). For example, quality control technology stimulates the development of Artificial Intelligence through the control of the parameters optimization. In turn, in solving complex quantum problems an important issue is connected with large-scale quantum devices, namely the effective optimization of

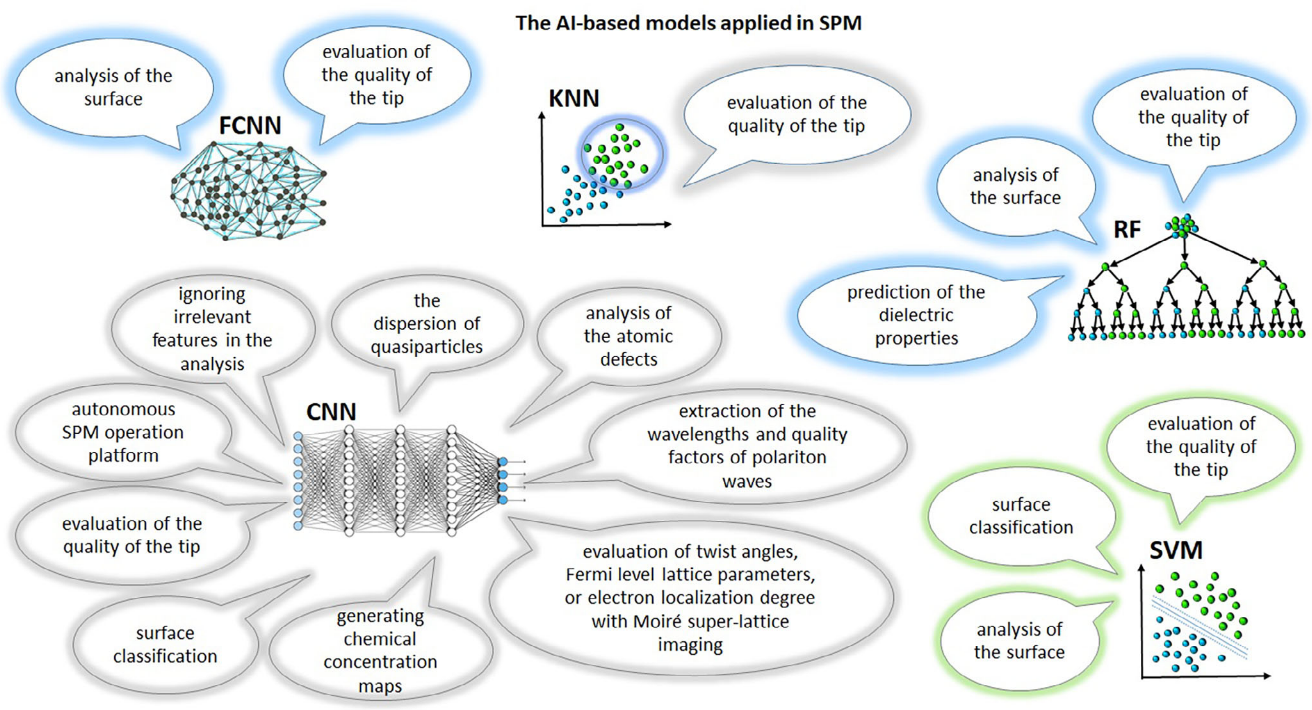

FIGURE 3 The AI-based models applied in SPM (Krull et al., 2000; Azuri et al., 2021; Duan et al., 2021; Xu et al., 2021; Mozaffari et al., 2022; Peng et al., 2023; Rashidi & Wolkow, 2018; Kingma & Ba, 2014; Alldritt et al., 2022; Carlson et al., 2015; Zhu & Yu, 2023; Zhang et al., 2018; Guo et al., 2021; Flöther, 2023; Larocca et al., 2023).

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TABLE 2 The comparison of the AI-based algorithms applied in scanning probe microscopy.

Application field	Accuracy (test sets)	Training/test sets [%]	Inputs parameters	Outputs parameters	References
Algorithm type: RF					
Recognition of the anomalies in the distribution of surface dangling bonds in the hydrogen-terminated silicon surface	0.89	80/20	3500 STM images (28 × 28 pixels)	Quality of the tip	(Rashidi & Wolkow, 2018)
Prediction of the dielectric properties of polymer nanocomposite interphases	0.94	84/16	200 finite-element simulations	Interphase permittivity	(Gupta et al., 2021)
Algorithm type: KNN					
Recognition of the anomalies in the distribution of the surface dangling bonds in the hydrogen-terminated silicon surface	0.84	80/20	3500 STM images (28 × 28 pixels)	Quality of the tip	(Rashidi & Wolkow, 2018)
Algorithm type: SVM					
Recognition of the anomalies in the distribution of the surface dangling bonds in the hydrogen-terminated silicon surface	0.88	80/20	3500 STM images (28 × 28 pixels)	Quality of the tip	(Rashidi & Wolkow, 2018)
Prediction of the dielectric properties of polymer nanocomposite interphases	0.94	84/16	200 finite-element simulations	Interphase permittivity	(Joseph & Farhadi, 2018)
Prediction of the dielectric properties of polymer nanocomposite interphases	0.92	80/20	200 finite-element simulations	Interface thickness and permittivity	(Gupta et al., 2021)
Algorithm type: MA					
Cancer diagnostics	0.99	66.67/33.33	SNOM images	Precise determination of oral squamous cell carcinoma	(Ellis et al., 2021)
Algorithm type: FCNN					
Recognition of the anomalies in the distribution of the surface dangling bonds in the hydrogen-terminated silicon surface	0.78	80/20	3500 STM images (28 × 28 pixels)	Quality of the tip	(Rashidi & Wolkow, 2018)
Segmentation of movable nanowires	0.90	about 80/20	220 AFM images of silver nanowires (112 × 112 pixels)	Representation of the nanowires in the form of a polygonal line	(Bai & Wu, 2021a)
Algorithm type: CNN					
Recognition of the anomalies in the distribution of the surface dangling bonds in the hydrogen-terminated silicon surface	0.97	80/20	3500 STM images (28 × 28 pixels)	Quality of the tip	(Rashidi & Wolkow, 2018)
Recognition of the spatial configurations, identification of the underlying Hamiltonian from a single domain configuration	0.99	80/20	Scattering scanning near-field infrared microscopy (SNIM) images	Hamiltonian	(Basak et al., 2023)
Algorithm type: CNN You Only Look Once version 3 (YOLOv3) (Moret-Bonillo, 2015)					
Segmentation of movable nanowires	0.90	about 80/20	220 AFM images of silver nanowires (112 × 112 pixels)	Representation of the nanowires in the form of a polygonal line	(Bai & Wu, 2021a)

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TABLE 2 (Continued)

Application field	Accuracy (test sets)	Training/test sets [%]	Inputs parameters	Outputs parameters	References
Generation of STM images of exfoliated 2D materials	0.90	90/10	170 black/white images (64 × 64 pixels)	Systematic database of STM images obtained using DFT	(open database, 2023a)
Data acquisition, the algorithmic search of good sample regions, evaluation of the condition of the probe	0.94	76/24	7589 constant-current STM topography images (64 × 64 pixels)	Condition of the probe, appropriate action location, identification and rectification of probe contact loss/crash incidents	(Krull et al., 2000; open database, 2023b)
Algorithm type: CNN + SVM					
Classification of super-resolution enhanced chromosome images	94.6	70/30	5474 images of chromosomes (64 × 64 pixels)	Classified super-resolution enhanced chromosome	(BioImLab, 2023; Menaka & Vaidyanathan, 2023)

parameters of a large number of components, while the complexity of quantum states and dynamics increases potentially with their system size (Moret-Bonillo, 2015). It is especially important in the context of the SNOM extension to the light frequencies, that is, the THz spectral region (Zhang et al., 2018). As a consequence, the analysis of the local electro-optical changes in real space in time and emerging quantitative phases in the THz range is obtained (Guo et al., 2021). This solution enables a non-invasive and even almost contactless measurement technique that is dedicated to materials of low-frequency conductivity (in the nanoscale) with high temporal resolution. This leads to the efficient evaluation of material properties like for example, low-energy resonances, or non-dissipative conductivity peaks towards zero frequency (Luo et al., 2023). However, Artificial Intelligence uses huge amounts of data for calculations, the processing of which requires significant hardware resources. Thus, quantum Machine Learning (QML) combines AI with quantum computation to develop algorithms for pattern recognition based on the advances of quantum computers like parallel computations and the application of quantum entanglement to perform computations. The first attempt in this field has been made by introducing quantum neural networks (QNNs) (Flöther, 2023). This type of neural network used in computation processes the quantum circuits (Junyu et al., 2023). In Reference Larocca et al. (2023), the concept of soft quantum perceptrons (the parameterized quantum circuit with the adjustable parameters of the quantum gate) was introduced. The quantum bits are calculated among others based on the superposition of the state, entanglement, and interference (Sim et al., 2019). It turned out that this approach has a nonlinear classification ability compared to the classical perceptrons. The comparison of the performance of AI-based algorithms in SPM is summarized in Table 2 and different AI-based models or tools and flowcharts are presented in Figure 4.

The AI enables a continuous operation of SPM without human supervision. The algorithm is able to make decisions regarding further steps and oversee the whole data acquisition process. An interesting example of ML-based autonomous SPM operation relies on a search of surface regions of interest, CNN assessment of the image quality and deep reinforcement learning agent assessment of the probe quality (Krull et al., 2000). DeepSPM can perform autonomously continuous data acquisition following the routine: first, the algorithm approaches the oscillating metallic tip to the surface, searches for promising regions and performs scans, determining the measurement parameters. Then, DeepSPM algorithmically evaluates the image quality and verifies if the contact between probe and sample is lost—if the state is deemed as good, a supervised learning trained CNN classifier evaluates the state of the probe by analyzing the obtained scan and predicting the probability of it being measured with a crashed probe. If everything is good, it stores the image and moves the probe to the new site to perform the next measurement. In case of a bad probe, a deep reinforcement learning agent, controlled by a second CNN, conditions it on the basis of list of predefined actions (e.g., applies a voltage pulse between probe and sample, dips the probe into the sample). Each conditioning step is followed by a measurement assessing the outcome. The optimal conditioning procedure is forced by cumulative

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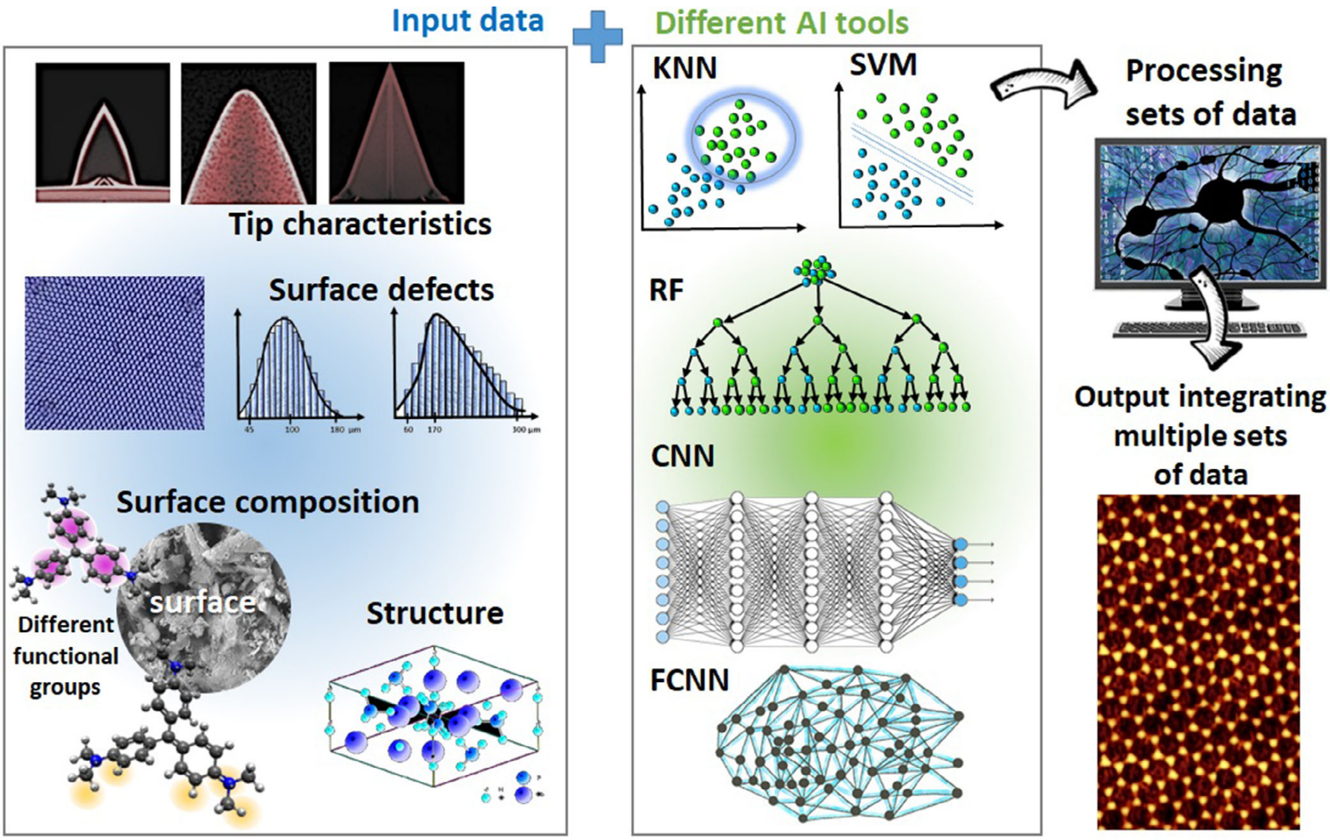

FIGURE 4 Different AI-based models/tools and flowcharts for SPM.

positive and negative rewards based on Q-learning. In case of a defective acquisition (lost contact, bad sample region) DeepSPM moves the probe macroscopically over a long distance to the new site, reestablishes contact and performs new measurement. Similarly, a ML-driven automated SPM scheme can be applied in ferroelectric materials research in Piezoresponse Force Microscopy (PFM) (Liu, Kelley, Vasudevan, Funakubo, Fields, et al., 2022b). A Deep Kernel Learning (DKL) framework assesses the relationship between the domain structure and polarization switching or nonlinearity in real time. Then, a hypothesis-learning scheme (Liu, Morozovska, Eliseev, Kelley, et al., 2023a) allows for autonomous identification of local bias-induced domain switching and test model hypotheses within the smallest number of steps. Then, the system maps large areas and identifies the interesting objects, followed by automated detailed scans of those objects. AI can be also used as a tool for automatic particle recognition and characterization for STM. U-Net network with EfficientNet-b3 network allows to avoid tedious manual counting and measuring particles' size (Liz et al., 2020). Another interesting application of AI is automatic functionalization of AFM probe with CO molecules (Alldritt et al., 2022). The algorithm based on CNN is able to recognize CO molecules in a single image and guide the tip to collect the molecule from the Cu(111) substrate. Subsequently it connects with microscope software to adjust the tip properly under the objective and performs the STM scan of other CO molecules on the substrate and uses those scans as an input to assess the centeredness of the CO molecule with respect to the tip. The characteristic sombrero-shaped features allow for a clear distinction of CO from other molecules and assess the symmetry of the tip-CO molecule system. Then, based on a tip quality, the decision is made whether the functionalization procedure needs to be repeated or the tip is ready to perform the proper measurement. Also, the simulations of working AI controller based on Double Deep Q-learning technique (DDQL) in AFM were presented (Degenhardt et al., 2024). The DDQL controller is trained on simulated AFM scans and adapts dynamically the control behavior. In normal situation it minimizes the root-mean-square (RMS) control deviations by a factor of 4 in comparison with PID controller. However, in situations when the cantilever tip is at risk, the AI-based controller sacrifices the mathematical goal of lowest possible control deviations and prioritizes the tip and sample safety. In detail, the AI controller uses the value of oscillation amplitude of an AFM-AC tip to calculate subsequent motion commands in z direction for the closed-loop piezo scanner. In the initial training, 5 neurons from the input layer receive the last five measured values of difference between setpoint and measured oscillation amplitudes. The other five neurons receive the last five piezo stage motion commands. Six fully connected hidden layers calculate which one of the available motion actions in z direction is the best choice. During the actual training, the AI controller performs actions by itself and learns from their consequences, while the PID controller works as a backup, performing actions when the cantilever tip is about to lose contact or approach too close to the surface.

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Usually, the sample surface sites that are of interest to researchers (like defects, vacancies, interfaces, impurities, etc.) are sparse. The possibility to direct the SPM tip to one of the desirable locations could significantly reduce the time and volume of data. To avoid time-consuming human assistance, autonomous search and acquisition techniques are developed. To obtain a fully autonomous data acquisition, the AI algorithm needs to control SPM apparatus and adjust scanning parameters in real time. A DNN framework can be used to realize fast automatic sample area selection based on a localization and shape detection of living cells (Rade et al., 2022) without the necessity to manually navigate to a spot before performing a scan and later retract the probe to manually move the tip to another spot for subsequent scanning. A transfer learning approach is applied to train the real-time object detection framework YOLOv3 algorithm to adapt the shape detection model to recognize particular shapes in low-quality AFM phase-contrast images. It is based on identifying and subsequent classification of the object (based on multiscale predictions) as well as predicting its position in a virtual grid. The algorithm assesses the probability of the object to belong to one of the predefined groups. Later, the optimal AFM piezo stage trajectory is generated and a closed-loop trajectory tracking control is utilized for high speed automatic navigation in x and y directions, with additional piezoelectric actuators for fine-tuning minute distances. Another method of autonomous experiment uses Gaussian process (GP) regression and a 1D CNN (Thomas et al., 2022) in scanning tunneling microscopy (STM) experiment for an identification of point defects in a variety of different surfaces. The method allows autonomous sample measurement at a low spatial density, which saves the operator time. The algorithm collects hyperspectral data, based on the spatial parameters and tip offsets in horizontal directions defined by an input image. GP defines the points where the tip is held at constant height and the bias is to be set over a defined voltage. Subsequently, the collected spectra are used in cross-correlation feature tracking with a trained model, that is, they are identified without any cognitive bias by 1D CNN, which calculates class probabilities and, subsequently, the sum of dI/dV signal is used in GP computations. In result, sufficient information can be obtained with around 1% of the data necessary in standard experiment. A framework based on GP and Bayesian optimization (BO) can be utilized in automated investigation of polarization dynamics in ferroelectric materials in piezoresponse force microscopy (PFM) or spectroscopy (PFS) (Vasudevan et al., 2021). A problem-specific tuned BO is used in real-time acquisition and pathfinding tasks during operation of SPM, which is possible due to edge computing on a GPU server. A single step of the GP-based BO process of the workflow encompasses: using Bayes rule to receive the distribution on the basis of a set of function evaluation; obtaining an acquisition function that allows to define the next move; defining most promising spots; performing scanning in the chosen spot, evaluate the obtained data and refine the function. This cycle of learning, choosing, evaluating, and refining helps the BO procedure efficiently find the optimal value of the main function. An incorporation of preacquired data or prior knowledge about the promising spots significantly improves the efficiency of the algorithm. Moreover, it is expected that quantum algorithms will especially change the modeling of nanostructural physical systems, where quantum laws play an important role. Although quantum machine learning is still in its infancy and can be treated only as an auxiliary tool nowadays, it would allow us to overcome physical constraints in ML algorithms and learn the complex behaviors, unobtainable for classical ML (Botifoll et al., 2022). The development of quantum algorithms promises a breakthrough in simulating physical systems where quantum mechanics plays a fundamental role. Since nanostructures inherently operate according to quantum principles, utilizing these algorithms would significantly improve the accuracy of their simulations. Working quantum system ProteusQ was shown by Qnami (QNAMI, n.d.). Diamond quantum technologies allow to measure nanoscale magnetic properties and AI deals with the problems of extracting important features from a large amount of noisy data sets and generalizes the information to use it for another data sets. This innovative ML algorithm revolutionizes quantitative magnetization reconstruction by delivering superior reliability and accuracy compared to existing methods (Dubois et al., 2022). The potential of the system can be extended with standard SPM modules, as AFM.

7 | SCANNING PROBE MICROSCOPY SUPPORTED BY ARTIFICIAL INTELLIGENCE AND QUANTUM COMPUTING—CHALLENGES

Since image acquisition and image analysis are not performed at the same time, a lot of unused data is produced (Caicedo et al., 2017). Additionally, the training data which are used by AI to train is usually prepared manually. This is a time-consuming and laborious task that is not free of human errors (Gordon et al., 2019). The resulting accuracy and reproducibility can limit confidence in the results' correctness (Schoppe et al., 2020). To reduce human error it is recommended that more than one expert labels training and validation data. Another known problem that occurs during training a machine learning algorithm is overfitting (Li et al., 2018; Sotres et al., 2021). It happens when the model does not generalize the obtained information and its interpretations are accurate only for the training data. It is a consequence of too small training data size (Liz et al., 2020), too noisy data (Corrias et al., 2023), underrepresented data (Li et al., 2020), too long training on the same dataset (Enke & Mehdiyev, 2012), or too complex a model that can take noise into account (Hu et al., 2021). Strategies to overcome this drawback include increasing the data sets (Lüder, 2021), transfer learning, that is, the knowledge gathered in the previous task is used in the next one (Rodani et al., 2023), cross-validation of the model performance on new data (Ito et al., 2018), regularization (data augmentation, which consists in modifying the copies of training data to artificially increase the training dataset (Caicedo et al., 2017), test-time augmentation, which increases and diverse the test dataset (Wang et al., 2019), random dropout of selected neurons during training (Liz et al., 2020; Xu et al., 2021), early stopping that ends training when the validation set is no longer improved with updated parameters (Pattison et al., n.d.; Ghosh,

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Sumpter, et al., 2021a; Wrzesiński & Markiewicz, 2020) or L1 and L2 regularizations that add a penalty term to the loss function to create unconstrained problems (Meldgaard et al., 2020; Miyama & Hukushima, 2018)), model selection (Li et al., 2018; Liu, Vasudevan, Kelley, Funakubo, et al., 2023b), prior probability distribution, that is, assessment of the result done before the experiment (Packwood & Hitosugi, 2017) or pruning the non-critical sections of the decision tree (Käming et al., 2021).

Besides, the AI technology complexity limits the possibility to understand and modify algorithms to adapt them to particular requirements (Carvalho et al., 2019). Currently, AI cannot surpass humans in the analysis of incomplete, multi-domain data, which are significantly different from the training data (Grudinin et al., 2023). Hence, due to a trade-off between accuracy and generalization, higher reliability in the case of different tasks is achieved with several specialized algorithms than with one versatile network (Ziatdinov et al., n.d.). The choice of the machine learning algorithm should align with the specific requirements and goals of the project to ensure effective and successful implementation. Selection of an AI-based algorithm for a particular application depends on the quality of data, training dataset size, number of features that need to be recognized, the necessity of human annotation, type of learning algorithm, type of network and their parameters, network topology, model complexity, speed and training time, memory requirements and balance between accuracy and interpretability of the results.

The AI-based method also entails the possibility of making mistakes due to training on historical data, which may be subject to operator error. Moreover, the experimental techniques are not efficient in terms of data set production. In fact, numerical calculations and experimentation increase the amount of data needed to develop accurate algorithms. This leads to another issue in application AI/ML-based methods and is connected with replacing static datasets with processes of active generation of data and employing autonomous systems (Ragone et al., 2023). However, they are not as risky in the case of SPM as, for example, in the case of autonomous cars.

Another important issue in the application of the AI-based system in the field of SPM in practice is cost and computational time. Thus, the combination of AI and QC has a huge potential to shorten the time needed to train and validate the neural network as well as the optimization processes (Valdez & Melin, 2023). Still, this union is challenging (Zhu & Yu, 2023), for example, for hardware and software incompatibilities. A majority of AI-based algorithms function on specialized graphical processors, while quantum computers are based on qubits that operate at low temperatures. All a joint common programming language is a challenge (the AI-based algorithms are written mostly in Python, while QC is in QASM). Other issues are connected with the low-performance levels of quantum computers and corrections of errors. Moreover, the problem of data security remains. For example, some quantum algorithms, although they are faster than classical cryptography methods, are not immune to "harvest now, decrypt later" attacks (Harishankar et al., 2023).

However, it is worth stressing that also the experimental evaluation of the AI, QC, and SPM integration is of high importance. Thus, the traditional SPM systems, that is, without AI and/or QC integration can be treated as a baseline. Evaluation of the system can be made in terms of a comparison of a number of factors, including resolution, measurement accuracy, speed, reliability, and the ability to detect defects or anomalies in samples.

8 | LIMITATIONS

The limitations of AI in SPM are that the complexity and noise of SPM data limit the inference of AI models. The first limitation may be very complex and noisy, containing various artifacts, surface irregularities, and environmental disturbances, which may lead to errors in analysis and interpretation by AI. The second limitation is connected with AI models trained on specific datasets that may not generalize to other cases. This may also contribute to the reduction of the AI-based algorithm's reliability in real-world SPM applications. Taking into account limitations of QC in SPM are connected with hardware constraints, namely qubit coherence times, gate fidelity, and scalability. In turn, quantum computing is susceptible to errors caused by noise, decoherence, and imperfect gate operations. These can be mitigated by implementing various types of data preprocessing techniques, including noise reduction, data denoising, and feature extraction. They can help improve the quality of SPM data that will serve as input data to the AI. Additionally, the development of error correction codes and error-tolerant techniques may increase QC potential. Given the current state of QC development, combining classical and quantum computing resources using hybrid algorithms and architectures may prove to be a good alternative. Mutual synergy can help overcome some of the disadvantages of both approaches and lead to improvement of the reliability and precision of SPM measurements.

9 | DISCUSSION AND CONCLUSIONS

The demand for three-dimensional insights through Scanning Near-field Optical Microscopy (SNOM) can be effectively met through AI-QC, particularly for nano-scale objects. By leveraging data from nano-scale structures or organic entities like viruses and bacteria, simulated environments can be constructed. This facilitates the conversion of two-dimensional SNOM images into corresponding 3D representations. To achieve this, established methodologies like multivariate static analysis (X) will be employed (Jin et al., 2017). These techniques not only capture structural attributes but also highlight plasmonic characteristics, a hallmark of SNOM methodologies, within the 3D models. Additionally, global datasets need to be systematically organized and integrated with experimental findings via AI algorithms to generate comprehensive three-dimensional models. However, the computational power required for these processes surpasses current capabilities, necessitating advancements in quantum computing (Yang, 2024). The pursuit of such computational prowess is vital for the continuous refinement and advancement of these methodologies.

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Thus, scanning probe microscopy is a versatile instrument that dramatically improves the resolution of surface examination up to atomic scale (Hui & Lanza, 2019; Wang, Lee, & Wei, 2023c). However, it is not a technique without flaws, the biggest ones include various types of artifacts that are important when interpreting the results obtained. In turn, the recognition of natural images using Artificial Intelligence is very advanced, however, the recognition of microscopic images causes problems because they contain a lot of noise and distortion (Gordon & Moriarty, 2020). A further concern is associated with the fact that microscopic images are in shades of gray. The data is also high resolution, that is, the data is more complex (larger) than natural image data. Thus, the application of Artificial Intelligence, in particular, deep neural networks in the field of scanning probe microscopy may contribute to a significant increase in the efficiency and accuracy of measurements (Caicedo et al., 2017). It can provide an understanding of the material's structures on a level not yet available to humans (Patton et al., 2018; Zhang et al., 2019). While the interaction between the tip and the surface is approximate with the simplified geometry, the AI has a huge potential to predict the essence of the correlation between the signal and the properties of the sample. In turn, the AI-based algorithms can actively select subsequent scan regions based on the output data and predefined acquisition function and thus contribute to improving the selection of scanned areas (Liu, Vasudevan, Kelley, Fudnakubo, et al., 2023b). Algorithms should take into account all kinds of factors that can lead to bias in measurements, including differences in tip geometry (length, tip radius, shape, and wear) (AlQuraishi & Sorger, 2021; Ghosh, Nachman, & Whiteson, 2021b). Another important issue, when developing the computation tools is proposing a high-accuracy method where there is no need to threshold grayscale images.

The comparison of the AI-based algorithmic performance in the field of SPM taking into account algorithms type, their application field, accuracy, the proportions of training sets to test sets, as well as inputs and outputs parameters, has been done in Table 2. It turned out that AI methods in the areas of the SPM are mostly concentrated after the extraction of structural information. The convolutional neural networks provide high accuracy, that is, above 90.00 percent in the various types of tasks, including tasks relying on the recognition of the anomalies in the distribution of surface dangling bonds in hydrogen-terminated silicon surface (Rashidi & Wolkow, 2018), segmentation of movable nanowires (Bai & Wu, 2021b), classification of super-resolution enhanced chromosome images (Menaka & Vaidyanathan, 2023), evaluation of the condition of the probe (Krull et al., 2000), tip conditioning (Wang et al., 2021) and even generation of STM images of exfoliate 2D materials (Basak et al., 2023). While techniques like K nearest neighbor, Random Forest, and Support Vector Machine enable achieving lower accuracy given the same set of inputs. On the other hand, generative models are also applied to evaluate the correlation between the input data and the output data (Ge et al., 2020). On the other hand, one of the limitations of using Artificial Intelligence in AE seems to be that it requires a lot of computing power compared to the processing of typical data and data acquisition times (Gongora et al., 2023; Krull et al., 2000; Thomas et al., 2022). Thus, automatic image recognition combined with experimental measurements gives benefits such as saving time, minimizing errors, and the ability to analyze data with precision not available to the human eye (Li et al., 2022). Since Artificial Intelligence requires a large amount of data (Yao & Chen, 2023), however, experimental measurements are time-consuming, and very often theoretical calculations and simulations based on their results are used to develop data that can enlarge the required databases. Also, platforms and libraries that enable the automatic analysis of images at the atomic level are slowly emerging, such for example Atomvision (Choudhary et al., 2023).

The important issue concerning AI-driven approaches is connected with the adequacy and diversity of datasets. Thus, the variability present in materials science applications that can be beneficial from SPM should be covered, namely the datasets should represent a wide range of material compositions, surface properties, defect types, and experimental conditions encountered in SPM. Counteracting various types of bias in data is also an important element. In turn, to ensure this convergence one can apply the data augmentation techniques. For example, introducing changes to sample properties, such as surface roughness, defect size, or chemical composition. Another possibility is to apply transfer learning, that is, using pre-trained models or knowledge from related domains can speed up model training and improve performance. Moreover, in the area of neural network learning, continuous learning can be applied (Zhu et al., 2024). This allows them to adapt to new data and evolving experimental conditions, ensuring their relevance and effectiveness over time. Another approach is to apply the selection of data sets specific to those important from the point of view of a specific material. AS a consequence, AI algorithms will capture only relevant features and differences inherent in SPM measurements.

One of the future directions of research is the development of generative Artificial Intelligence, which can enable the formulation of answers in the natural language regarding the course of microscopic measurements and samples in the SPM (Kalinin et al., 2023). It also can contribute to the creation of next-generation intelligent laboratories for functional nanomaterials (Peng & Wang, 2023). The first attempt has been made in the fields of AFM automation, in particular, data collection (Dujardin et al., 2019; Szeremeta et al., 2021). On the other hand, the development of tools for effective analysis of texts, in particular scientific texts, will also enable the creation of structured databases (Tshitoyan et al., 2019). Another research line is connected with the development of methods for reliable assessment of measurements carried out by non-specialists. However, the key to improving the overall understanding of the process of scanning probe microscopy and the mechanisms that govern it is to combine the experiment with its numerical simulations and support it with AI-based tools.

Thus, Artificial Intelligence, with its capability of modeling and analyzing the results and comparing them with a constantly growing database of measurements, increases the credibility of the new results obtained with SPM. Nowadays, the possibility to use AI resources has significantly expanded the capabilities of scanning probe devices, improving the reliability of their results by eliminating errors coming from ignorance and experiments. The theoretical output obtained from AI models can be correlated with experimental data and

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introduced into the device control system to obtain more trustworthy models. Thus, integration of the SPM technique with Artificial Intelligence-based algorithms offers the potential to eliminate most of these measurement technique flaws, especially those associated with artifacts or human factors. This integration significantly enhances the process of sample analysis (Gregoire et al., 2023). It also enables an autonomous system operation to optimize and acquire data without on-site supervision (Wu et al., 2018). To summarize, the results obtained indicate that both modeling and the use of Artificial Intelligence-based algorithms, in particular Machine Learning techniques, can significantly improve scanning probe microscopy and data interpretation processing (Ragone et al., 2023). The proposed approach can be applied in molecular diagnostics and screening applications. The simulations can offer an understanding of the fundamental physical and chemical principles governing the behavior of materials. In turn, AI-based methods can enable probabilistic learning of atomic interactions. In addition, natural language processing (NLP) can also help organize and classify knowledge in the context of SPM by searching for key information in the literature. Moreover, the combination of Artificial Intelligence and quantum computation may be a benefit, however, both require significant improvement (Melnikov et al., 2023; Qin et al., 2023). Thus, the tensor network systems that transmit and process a huge amount of information seem to be implemented in the future in almost every area of life.

Quantum computing is a promising alternative to classical computers due to its ability to perform certain calculations exponentially faster. However, the feasibility of integrating quality control into SPM systems is currently limited by hardware limitations, error rates, and the complexity of quantum algorithms. Quantum Machine Learning (QML) can be used to analyze and classify SPM data more efficiently than classical machine learning approaches. For example, quantum support vector machines and quantum neural networks may have the potential to infer large data sets with greater accuracy and speed (Kimoto et al., 2024). Another QC feature that can accelerate materials discovery and optimization processes, reducing the need for time-consuming and expensive experimental trials is quantum simulation (Khajavi et al., 2024). It enables mimic and predict the behavior of complex materials. Also, quantum optimization algorithms like quantum annealing and variational quantum algorithms are very promising. They can be applied in various tasks, including image reconstruction, feature extraction, and pattern recognition, optimizing the measurement process and improving the resolution and sensitivity of SPM techniques. Despite the above-mentioned advantages, QC also has disadvantages such as hardware scalability, error mitigation, and designing quantum algorithms that are tailored to specific requirements. The latter will be crucial to realizing the full potential of quality control integration.

10 | FUTURE PLANS

One of the most promising research directions appears to be the development of algorithms that harness the power of quantum computing to efficiently analyze large experimental datasets generated by SPM, including Quantum Machine Learning algorithms. Combining AI and QC in this context and developing adaptive control algorithms that optimize scanning parameters based on feedback from quantum sensors and classical data analysis represents the next frontier of research. This could be extremely beneficial, for instance, in predictive modeling of nanoscale processes and automated decision-making to optimize experimental parameters in real-time. Additionally, the application of quantum simulations in the case of nanoscale systems may enable more accurate modeling of atomic and molecular interactions, thereby leading to more precise predictions of the behavior of nanoscale materials under various conditions.

Another research direction is linked to advancing generative Artificial Intelligence systems. These systems hold the potential to articulate responses in natural language concerning the progression of microscopic measurements and samples within SPM experiments.

It is worth mentioning that a key issue is to foster cooperation between fields, particularly informatics, physics, materials science, and others. Financing joint (cross-field) research initiatives appears to be a positive step. Similarly, providing resources and infrastructure to support interdisciplinary projects focused on integrating artificial intelligence, quantum computing, and SPM could yield significant progress. Organizing various scientific events where researchers from different fields can exchange ideas, share observations, and identify common research interests may also be beneficial. Moreover, ensuring open access to data and resources is crucial for developing effective Artificial Intelligence methods, regardless of the field.

AUTHOR CONTRIBUTIONS

Agnieszka Pregowska: Conceptualization; investigation; writing – original draft; methodology; writing – review and editing; supervision; resources; data curation; formal analysis. **Agata Roszkiewicz:** Conceptualization; investigation; writing – original draft; methodology; writing – review and editing; formal analysis; resources; data curation. **Magdalena Osial:** Investigation; writing – original draft; visualization; methodology; formal analysis. **Michael Giersig:** Conceptualization; writing – review and editing.

DATA AVAILABILITY STATEMENT

Data sharing not applicable to this article as no datasets were generated or analysed during the current study.

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