Leveraging Large Language Models and Social Media for Automation in Scanning Probe Microscopy

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We present the development of an automated scanning probe microscopy (SPM) measurement system using an advanced large-scale language model (LLM). This SPM system can receive instructions via social networking services (SNS), and the integration of SNS and LLMs enables real-time, language-agnostic control of SPM operations, thereby improving accessibility and efficiency. The integration of LLMs with AI systems with specialized functions brings the realization of self-driving labs closer.

As the level of sophistication and reproducibility required for experiments increases, it becomes more difficult to master the experimental equipment. This situation implies the need for methods and tools to facilitate experiments. One way to address this problem is through the use of artificial intelligence (AI) and its integration into experimental instruments[1–4]. In particular, there is widespread interest in creating an environment of automated solutions[5,6]. On the other hand, the implementation of fully autonomous systems in experimental research is still in its infancy, despite the promise of revolutionizing research by automating routine tasks and analyses. It will still take time for individual researchers to obtain an environment in which they can implement specific experimental AI themselves[7–11]. As an alternative trend, research on the use of generative AI[12] in experiments is gaining traction. Generative AI's capability to create complex data patterns and processes is desirable in increasingly intricate experimental procedures[13–16]. Among various types of generative AI, large language models (LLMs) stand out for their potential to act as cognitive mediators between researchers' objectives and general tasks. Thus, LLMs can be transformative tools, enhancing the efficiency and accessibility of user and experiment instrument interactions. In this manuscript, we present the use of an advanced LLM in scanning probe microscopy (SPM) experiments, functioning as a measurement agent. This SPM system is designed to receive and process instructions via social networking services (SNS), enabling real-time, language-agnostic control of SPM operations.

Figure 1 shows an SPM system integrated with LLM and SNS. Our system integrates a front-end SNS client utilizing Slack web app[17] for receiving user commands, and a back-end embedded system for command processing and execution. To deal with user actions, we utilize Slack API's event subscription feature, allowing the system to listen to the user messages that are sent to specific Slack channels. User messages can be in multiple languages, and different message types (text/audio). The SPM agent involves translating user commands into

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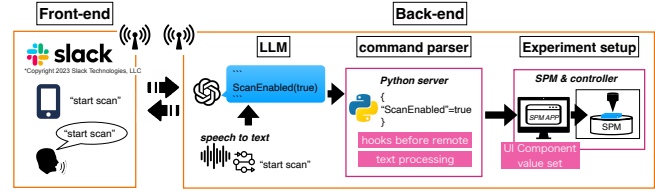[a)]enzian0515@gmail.com
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FIG. 1. Schematic diagram of interactive system of scanning probe microscopy (SPM). In the experiments, Slack, a social networking service (SNS), is used for the human input portion of the commands, which ChapGPT, a large-scale language model (LLM), understands and converts into actual commands for the SPM device.

executable SPM commands via a sophisticated AI model that processes natural language and speech inputs, leveraging OpenAI's Whisper[18] for speech-to-text (TTS) conversion and ChatGPT (gpt-4-0124-preview)[19] for understanding and generating appropriate commands for SPM control (text-to-command: TTC). The system's core, a Python server, hosts the custom SPM controller, facilitating direct TCP connection with the SPM instrument. The SPM controller can receive commands in JSON format to set the value of the corresponding UI element name. In Fig. 1, as an example, for a switchable UI named "ScanEnabled", giving it a true value will control the SPM to start scanning.

Constructing clear and detailed LLM prompts regarding parameter settings and behavior in the experiment is important for the LLM to make the following decisions from the incoming messages. The following prompt is an example of a configuration in our system.

"You are a robot controlling a scanning probe microscopy. Users will provide instructions in text format on how to control the device, and you'll need to translate these texts into specific programmatic commands. " , "You can control and set the scan parameters in the scanning probe microscopy. " , "The below list shows the function about what you can do. Each programmatic command is followed by parentheses containing the names

of required parameters. Following this is a description of the command, arg type indicates the type of parameter, and arg description represents the parameter's description." + command str, *"You should try your best to understand the instructions and use the list up functions to write. The function argument should follow the type I defined.", "If the user's instructions can be accomplished by multiple step commands, then output them sequentially and separate each command with a new line.", "If the user's instructions cannot be carried out by the commands provided above alone, please respond with 'None' first and then give a reason to user. Otherwise, reply with the names of the corresponding programmatic commands and provide appropriate values within parentheses. ", "Reply to me in language str."*

In the experiment, ChatGPT determines the instructions sent to SPM based on these prompts as well as five previous message histories and the current user message. "language str" will be replaced with the detected language name of the user message. This ensures that our measurement agent replies to the user in the same language they used. Table I shows the SPM experiment commands currently understood by the SPM agent. These commands are saved in a bulleted format, such as a CSV file so that they can be easily added or deleted. The bulleted command list we used in this paper is shown in Tab. I. In the above prompts, ""command str" will be replaced with the text content of this bulleted list. The table serves as an API reference documentation for the LLM, informing the supported SPM control command and explaining the usage of the commands and their arguments.

The output text generated by ChatGPT is then processed via a command parser, which converts it into a canonical format of the SPM command. Given the inherent uncertainty in AI-generated output, the command parser ensures that the resulting command line for controlling the SPM device adheres to the system's specifications. Unsupported output content is disregarded, while supported programmatic commands and their corresponding arguments are extracted.

Using the above-mentioned system, we perform the STM experiment operated in ultra-high vacuum condition ($< 1 \times 10^{-8}$ Pa) at room temperature. Mechanically etched PtIr STM tips (UNISON P-50 Pt; Ir) were used for imaging. As a sample, we prepare Si(111) clean surface by a standard flashing-and-annealing method. For data acquisition, we have established an SPM system built with LabVIEW, LabVIEW FPGA, and Python. NI PXIe-7857R was used as the measurement board, The scanning and data acquisition were controlled with Python script in which automated SPM measurement routines and scan functions for optimizing experimental

TABLE I. Description of Programmatic Commands for ChatGPT. Descriptions in the table is input to "command str" in the prompt.

Programmatic Commands	Description	Arg Type	Arg Description
StageOffset_X (arg)	Setting the absolute X (left and right direction) position coordinates of the probe (SPM tip)	float	Coordinate value of X in nanometers
StageOffset_Y (arg)	Setting the absolute Y (up and down direction) position coordinates of the probe (SPM tip)	float	Coordinate value of Y in nanometers.
StageOffset_X_ADD (arg)	Sets the relative X (left/right direction) position to be moved from the current coordinates of the probe (SPM tip)	float	Distance to be move in X, in nanometers
StageOffset_Y_ADD (arg)	Sets the relative Y (up/down direction) position to be moved from the current coordinates of the probe (SPM tip)	float	Distance to be move in Y, in nanometers
Sample_Bias (arg)	The bias voltage add to the measured sample	float	the value of the sample bias
Aux1MaxVoltage (arg)	Setting the scanning area range of the X size	float	scan range of the X direction in nanometers
Aux2MaxVoltage (arg)	Setting the scanning area range of the Y size	float	scan range of the Y direction in nanometers
ScanEnabled (arg)	Switches to control scanning	bool	true to start the scan and false to stop the scan

environment were contained.

Figure 2 shows a demonstration of STM measurements of the $Si(111) - (7 \times 7)$ surface using SNS. In part (A) of the figure, the operator inputs the incomplete English phrase "start scan 22.5 nm x 22.5 nm," intending to mean "Start scanning in the area of $22.5nm \times 22.5nm$". The backend system interprets the messages and sends the command (as shown in (B)) to the SPM. Here, 0.6V is the calibrated voltage value of the scanner equivalent to 22.5nm. Thus, even if the English are not perfect, the correct command is sent, thanks to LLM. Part (C) and (E) show that the SPM agent sends information messages indicating that scanning has started and finished, respectively. After the measurement, the scanned image is sent back to the operator as shown in (D). The image is filtered for easier viewing.

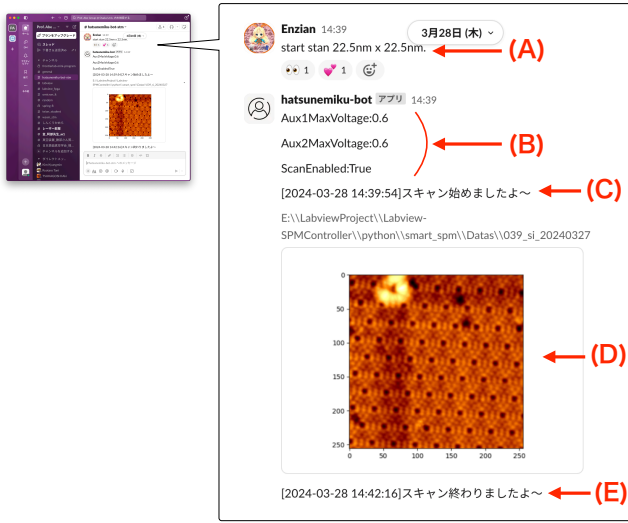Figure 3 shows the results of the experiment follow-

FIG. 2. An example of an STM experiment using SNS.

FIG. 3. The messages for image acquisition and responses in succession.

ing those presented in Fig. 2. As the STM image from Fig. 2 depicted an adsorbed object in the upper left portion, to avoid the ares, a message "shift in the y-direction by 5 nm" was entered as shown in Fig. 2 (a), then the tip positioning update was performed by 5 nm. Figure 3(b) confirms that the scanning avoided the adsorbed object by restarting the scan. In Figure 3(c), a message "set bias voltage to -2V and start scan" was input, setting the bias voltage to -2 V and beginning the scanning of 22.5 nm × 22.5 nm area. Since this negative bias was applied, both faulted and unfaulted half-unit cells are distinguishable. These steps illustrate that the two commands (changing the bias voltage and initiating scanning) were executed correctly. Although the scanning area was not explicitly mentioned in Fig.3(c), ChatGPT presumed the previously used scanning range as acceptable based on the command history and proceeded with the scan. In Fig.3(d), a message meaning "Start scanning in the area of 10nm × 10nm" was entered in Chinese. In the STM images on Slack, the start position of scanning is the upper left. Comparing with Fig. 3(c), we can see that the 10 nm × 10 nm area in the upper left portion is imaged. Additionally, Figure 3(e) shows a message entered in Japanese to scan a 22.5 nm × 22.5 nm area, resulting in the same image as seen in Fig.3(c). This demonstrates that, although the ChatGPT prompt is written in English, the LLM can interpret and execute commands in multiple languages.

According to the prompts, when ChatGPT judges the user message as "not executable", our system will extract the reason part from the generated text and send it to the Slack client. Figure 4 shows a result when a command not in Tab. I is entered into the message; the prompt instructs the user to answer "None" if the command cannot be executed and to tell the user why, and the message that shows the reason will be generated.

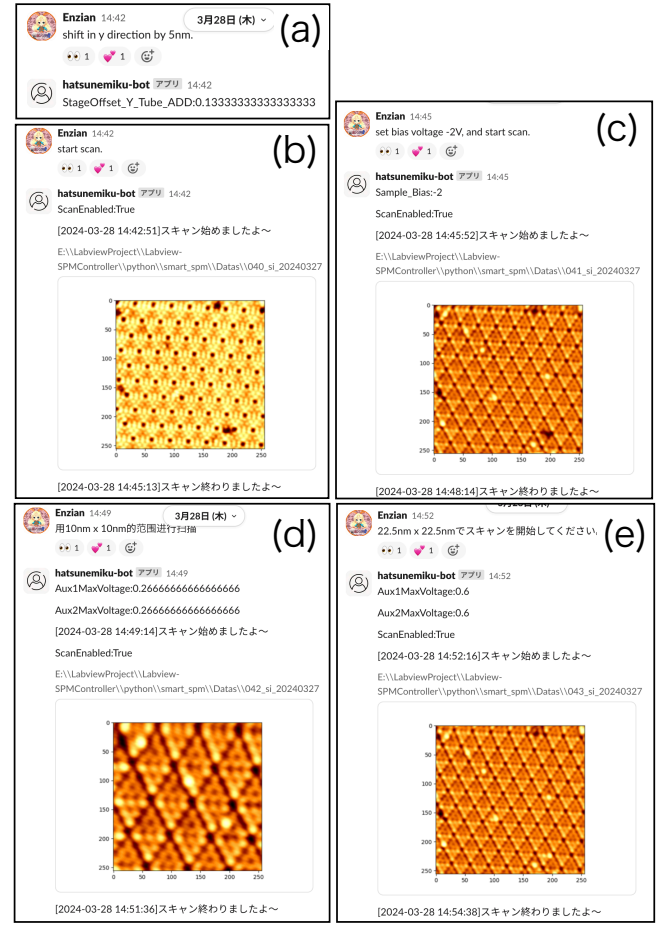This study has presented the stage for a detailed dis-

cussion of the integration of AI into the experimental process, exploring both its potential benefits and challenges. One of the primary goals of AI in scientific experiments is to realize a self-driving lab: to enable AI to perform preset experiments autonomously. On the other hand, depending on the research (for example imaging with microscopy), it will be necessary to check the results of the experiments in real-time. In such cases, humans will intervene in the experiment, but even then, they will always be constrained by the time it may take to check reproducibility and the experiment itself. SPM often requires not only skilled experimental techniques but also a very long time for data acquisition. In particular, while in spectroscopic measurements and atom manipulation experiments, it is essential to set up areas and parameters that allow appropriate data acquisition[20,21]. In such experimental studies, adding human guidance is an effective way to perform effective experiments and provide feedback to train AI systems capable of autonomously performing experiments. SPM operators have been dominated by manual and often labor-intensive processes[22–24]. As the complexity of experiments grows, so too does the challenge of mastering intricate methodologies, particu-
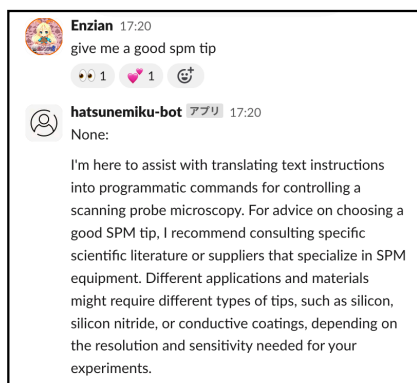
FIG. 4. Response from the SPM agent when a message related to a command that has not been preconfigured is sent.

larly for novices in the field. This underscores a critical need for innovative solutions that can streamline the experimental process and make high-quality research more accessible and reproducible.

The use of SNS and LLM proposed in this study is one way to solve these problems. As a prospect, LLM is expected to be utilized in a wide range of experimental applications. A general-purpose LLM such as ChatGPT could serve as the "brain of an experimental system" coordinating with other specialized algorithms and AI models to handle complex, specialized research tasks. The specialized AI model can extract features from the data in a higher-dimensional space compared to the model output[25,26](e.g., classifying a 256×256 pixel SPM image into a few labels of feature data, which will make LLM easier to understand). This feature information can then be incorporated into user prompts, allowing the LLM to determine the next experimental procedure using predefined prompts. Then, LLM can perform efficient experiments using more advanced SPM features, after we implement these methods into the system and enrich the method description in the document file of Tab. I. For example, to perform the automated SPM experiments, several advanced algorithms and AI implementations for SPM can be integrated into the system, including data processing methods[27,28], drift correction[29], tip reconstruction[10,30], and atom manipulation[31].

The accuracy of the AI can be improved by generating more detailed prompts, similar to instruction manuals. Fortunately, the "gpt-4-0125-preview" model supports up to 128,000 tokens, and given that a single conversation typically utilizes only around 500 tokens, the full potential of ChatGPT is not yet being leveraged. The AI can facilitate more advanced experimental operations by incorporating detailed instructions in the experimental apparatus into the prompts.

In summary, we have developed an SPM agent representing an innovative application of AI in scientific research, offering a user-friendly and efficient method for conducting SPM experiments remotely. This work con-

tributes to the broader efforts in automating scientific research, promising to accelerate experimental workflows and facilitate remote experimentation in various scientific fields.

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