

Materials science for quantum information science and technology

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Quantum computing, sensing, and communications are emerging technologies that may circumvent known limitations of their existing traditional counterparts. While the promises of these technologies are currently narrow in scope, it is possible that they will broadly impact our lives by revolutionizing the capabilities of data centers and medical diagnostics, for example. At the heart of these technologies is the use of a quantum object to contain information, called a quantum bit or qubit. Current realizations of qubits exist in a broad variety of material systems, including individual spins in semiconductors or insulators, superconducting circuits, and trapped ions. Further advancement of qubits requires significant contributions from materials science in areas of materials selection, synthesis, fabrication, simulation and characterization. Here, we discuss some of the needs and opportunities for contributions to advance the fundamental understanding of materials used in quantum information applications.

Introduction

Quantum information systems have attracted great interest in recent years. Research and development funding is increasing worldwide from both government and corporate sources. Technology opportunities have been studied by a number of organizations,^{1–3} and have motivated major government programs.^{4,5} The interdisciplinary nature of this technology and the ubiquitous importance of materials provides numerous opportunities for practitioners of fundamental and applied materials science and engineering to contribute needed advances. This article focuses on materials science applied to quantum information science and technology (QIST)—what we call “materials for quantum”—which is separate from the study of “quantum materials,” or those materials where quantum effects produce emergent behavior.⁶ While we attempt to provide perspectives on materials for quantum across a broad spectrum of QIST and to review the relevant major issues and technology trends, inevitably this article is not comprehensive, and we encourage the interested reader to consult the cited articles for additional details.

The science of quantum information has made significant advances from its initial concept in the early 1980s, when

Richard Feynman and Yuri Manin postulated that simulating quantum systems would be better done with a computer that is quantum mechanical.^{7,8} In the context of quantum information, this concept has evolved into the goal of using quantum mechanics to redefine the structure of information, whether for computation, communication, memory, or sensing. Today, researchers do not foresee quantum information systems in every home. Rather, quantum information systems are being designed to extend the state of the art for tackling only the most difficult problems. The announcement that a 53-qubit quantum computer can outperform a classical supercomputer on a specially tailored problem demonstrates the not-too-distant promise of quantum computation as a potential quantum co-processor in data centers.⁹ Demonstrations of magnetic sensing using spin qubits in diamond are being developed that dramatically alter sensing capabilities, opening new areas of use, while developments of quantum communications networks are imagined, for instance, to provide more secure financial transactions and interconnectivity of quantum information.

Some potential advantages of a quantum information approach are apparent from a simple contrast with

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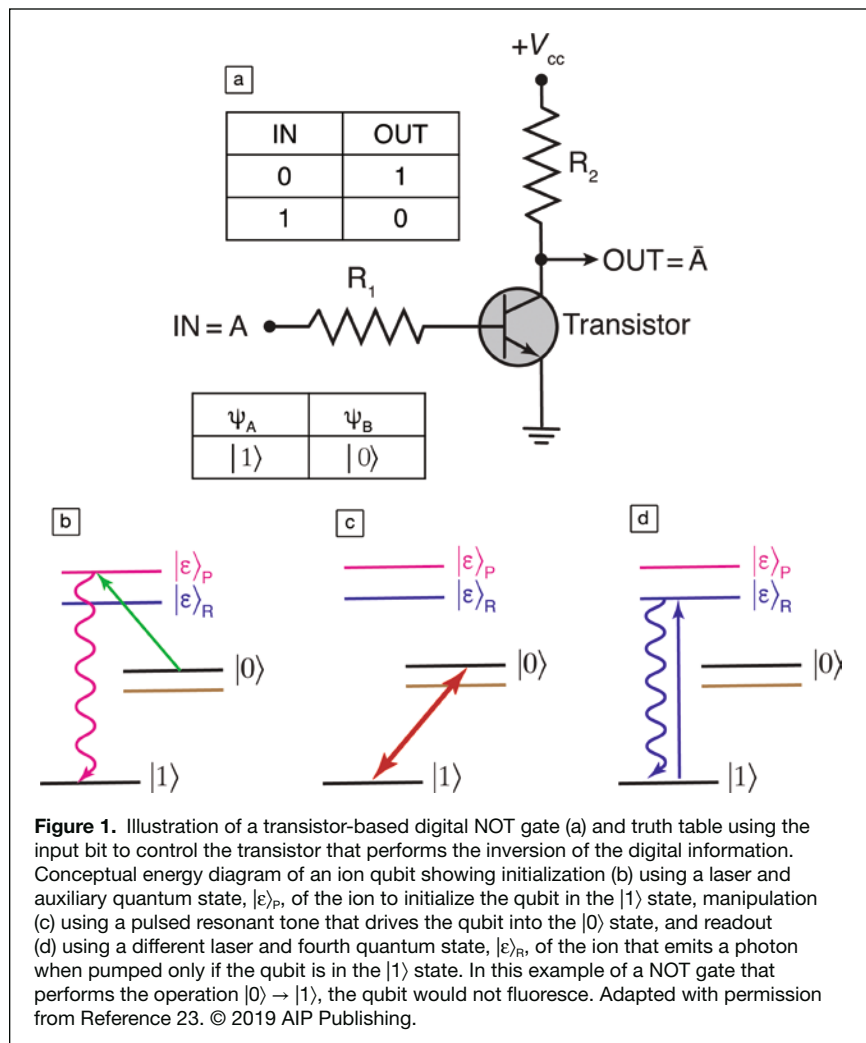


Figure 1. Illustration of a transistor-based digital NOT gate (a) and truth table using the input bit to control the transistor that performs the inversion of the digital information. Conceptual energy diagram of an ion qubit showing initialization (b) using a laser and auxiliary quantum state, $|\epsilon\rangle_P$, of the ion to initialize the qubit in the $|1\rangle$ state, manipulation (c) using a pulsed resonant tone that drives the qubit into the $|0\rangle$ state, and readout (d) using a different laser and fourth quantum state, $|\epsilon\rangle_R$, of the ion that emits a photon when pumped only if the qubit is in the $|1\rangle$ state. In this example of a NOT gate that performs the operation $|0\rangle \rightarrow |1\rangle$, the qubit would not fluoresce. Adapted with permission from Reference 23. © 2019 AIP Publishing.

classical digital information. Digital information is encoded in a sequence of binary digits, or bits, having the value 0 or 1. Individual classical bits are confined to encoding either 0 or 1 at an instance in time, enabling one of the strengths of digital information compared to analog signals. By contrast, quantum information is encoded in a quantum two-state system that not only can take quantized values $|0\rangle$ or $|1\rangle$, but also any complex superposition of these states. Furthermore, in contrast to analog information, where each bit is independent, quantum bits can be connected to each other through quantum entanglement. The uniquely quantum principles of superposition and entanglement provide for an enormous increase in information density and computational parallelism but come at the cost of needing to develop quantum analogues for bit operations, and to build these elemental operations up into algorithms for computation, communication, and sensing.

The DiVincenzo criteria¹⁰ (see sidebar) describe the requirements for quantum information. These requirements are similar to those for classical digital logic, but are complicated by having to contend with certain esoteric quantum principles, such as the inability to measure or copy a quantum

state without disturbing the state itself. In classical logic, where the digital states are usually voltage-based, setting and reading a digital state is as simple as setting or measuring the voltage at a node of a circuit. These voltage levels can be manipulated by sequentially cascading circuits together, but the function of each circuit is determined when the device is fabricated based on the layout of circuit components. For example, see the transistor-based NOT gate shown in **Figure 1a** that transforms the input bit (either a 0 or 1) into its opposite (either a 1 or 0) by using the input bit to turn the transistor on or off. In transistor circuits, the specific choices of the voltages and signal duration are engineered parameters that have seen dramatic changes during the history of transistor-based digital logic devices. Finally, high-speed operation is possible because the control is all-electrical, and the fidelity of these operations is high because voltage levels have a threshold for interpretation as 0 or 1.

The situation for qubits is significantly more complicated, as the quantum mechanical states represent the states themselves (e.g., the quantum mechanical ground state is assigned $|0\rangle$, and a selected excited state is assigned $|1\rangle$ instead of two simple voltage levels). Consider the simplified sketch of the electron levels of a single trapped ion that is shown in Figure 1. Initialization (Figure 1b) may use a specific laser to depopulate the $|0\rangle$ by using a third quantum state, $|\epsilon\rangle_P$, of the ion to initialize the qubit in the $|1\rangle$ state. Manipulation (shown in

Figure 1c) is accomplished with a pulsed resonant tone that can drive the qubit into the $|0\rangle$ state. Finally, the qubit can be read out (shown in Figure 1d) using a fourth quantum state, $|\epsilon\rangle_R$, of the ion that emits a photon, when pumped, only if the qubit is in the $|1\rangle$ state, and is dark in the $|0\rangle$ state. Each of these pulse frequencies is determined by the ion itself, not the circuit designer. However, the pulse durations and sequences of timed pulses can be engineered to manipulate the quantum states through a number of different logic gates using a single ion.

The desire to have precisely two addressable quantum states requires the use of systems that have non-degenerate energy levels that are well isolated. However, external manipulation of the states requires coupling to other degrees of freedom of the experimental system, counter to the idea of perfect isolation of the two-state quantum system. As illustrated in the example, initialization, readout, and manipulation require intricate experimental setups and extensive tuning of the quantum system—the very concept of two quantum states is a significant abstraction of these setups. The requirement for maintaining long lifetimes of the quantum states leads to involved cooling schemes such that the thermal energy is significantly lower than

Sidebar

DiVincenzo Criteria

David DiVincenzo outlined the basic system requirements needed to realize a quantum computer,⁹ which are rooted in classical information theory. These requirements have been termed the DiVincenzo criteria and consist of

1. A physical system implementing quantum bits (qubits), each with two well-defined quantum states.
2. The ability to initialize qubits to a known state (with high probability).
3. Manipulability of the quantum states with high fidelity to implement a universal gate set.
4. Long coherent lifetimes of the quantum states relative to the time needed to perform all of the desired manipulations.
5. The ability to read out the (final) state of a qubit with high fidelity.

For quantum computing, the essential nature of the criteria are nearly self-evident. They are rooted in the need for proper qubits to encode and maintain quantum states, along with the ability to execute prescribed transformations (algorithms) on those states to produce, in the end, a determined, measurable computational result. The ability to initialize the qubits to known states before a computation occurs relates to the ability to control a

computation so that the solution to a specific problem is found by the execution of the quantum program.

For quantum communication, the same criteria hold with two additional criteria added:

6. The ability to interconvert stationary and flying (transportable) qubits.
7. The ability to transmit flying qubits between specified locations with little decoherence of the quantum state.

While these additional criteria pertain specifically to quantum communications protocols that may require exchange of quantum coherent states and transmission of quantum information to third parties, they may also be considered optional criteria for quantum computing. In the context of computing, these additional criteria enable remote and distributed quantum computing paradigms, which may be important for modularization of quantum hardware.

For quantum sensing, many of these criteria remain valid; however, there is no need for a universal gate set. In addition, the manipulability criterion is best interpreted as a requirement that the quantum states evolve in a predetermined way in response to the sensing field, so that calibration of the sensor is possible. In a similar context, the ability to initialize, read out, and maintain sufficiently long coherence is clearly required to enable the function of the sensor.

the energy difference of the two quantum states. For computation, manipulation requires driving a controlled transition between the two states, often creating a superposition defined by two angular rotations and entanglement through a two-qubit gate. Finally, the requirement for fast manipulations requires strong coupling to a control field, while, paradoxically, the requirement of a long lifetime requires the system to be decoupled from its environment. Alternatively, for sensing, manipulation is the result of the sensing field that is coupled to the qubit.

A current recurring theme in quantum systems, spanning computation, communication, and sensing applications, is that they demonstrate low fidelity for initialization, manipulation, and readout, or they do not scale to large enough numbers of qubits to be practically useful. Drawing analogy to the materials-centric history of classical digital computing, quantum systems have yet to discover their silicon and silicon oxide—the material stack originally responsible for spawning the digital computing revolution—nor their hydrogen-forming gas anneal, which was the corresponding critical processing step that enabled the success of that material stack. In fact, in many cases, the identification of direct connections between some measurable properties of the physical system and quantum fidelity metrics remains an open area of research. Just as importantly, the ability to scale quantum systems to larger qubit counts remains challenging for a variety of reasons, both technological and practical—for example, the size and

complexity of the control systems or thermal isolation, or the inability to produce multiple qubits that behave the same and remain stable over time. Many of these problems, which prevent quantum systems from realizing a significant advantage over classical systems, are, at their core, problems that can be addressed with better materials. Explicating this connection requires more specific discussion about precise applications; in the following, we emphasize materials connections to quantum computation and quantum sensing.

Qubits and materials

An atom levitating in vacuum in the absence of all fields is what many students study in chemistry and physics courses as an ideal quantum system, yet it is a closed system and therefore not useable for quantum information. The failure to meet the basic DiVincenzo criteria becomes apparent, since it is impossible to initialize, manipulate, or read out the quantum state without interacting with the atom through some external field. A perfectly isolated system also cannot act as a sensor, since the essence of sensing is to interact with and report some external physical quantity or field. Therefore, the quantum systems that are useful as qubits are all open quantum systems. The surrounding environment influences open quantum systems, which is necessary for information applications, but unfortunately also allows noise to degrade the quantum mechanical state. This degradation affects the function of both

sensing and computing devices and often originates within the host materials that are used to create the qubit.

Selection of materials is an important first step in any technology. Undoubtedly for QIST, new materials will be introduced as the technology evolves, although the currently decided materials may persist indefinitely. Nevertheless, there are a number of engineering and fundamental contributions that materials science can make to QIST beyond materials selection. The most general contribution could be in understanding the properties of relevant materials in the environment that QIST devices operate. For example, the small energy scales of many qubit realizations (e.g., superconducting circuits, spins in semiconductors), combined with the requirements of the DiVincenzo criteria, drive engineering choices to operate QIST devices at the lowest possible temperatures achievable by current technology. Perhaps there will be materials advances that eliminate noise sensitivities and increase the relevant energy scales, thus allowing these computing devices to operate successfully at “elevated temperatures” such that dilution refrigerators are not necessary (temperatures above 300 mK). Alternatively, some qubit implementations (e.g., trapped ions, defect centers in diamond) can operate at room temperature even though they often are tested at low temperatures to maximize performance. It is safe to predict that most quantum-computing devices will operate in cryogenic environments for the foreseeable future, since eliminating thermal sources of noise is always advantageous. On the other hand, quantum sensors are often desired to operate at room temperature, so it may be assumed that many quantum-sensing devices will leverage qubit technologies operable in ambient laboratory environments for the foreseeable future.¹¹

For sensing, defect spin qubits in diamond have seen the greatest success. This success has largely been the result of the long coherent lifetime at room temperature. They have been incorporated into a large number of geometries leveraging both single and ensemble qubit sensors. While there is significant work in using entangled photons to create remote quantum sensors, we limit our discussions to the materials challenges facing defect spin qubits.

For communications, there is more than secure communications.¹² The accurate encoding of a pure quantum mechanical state that exists in a solid-state qubit, onto the pure state of a photon so that it can be transmitted to another stationary qubit, is a challenge with relevance to QIST broadly. Nevertheless, this type of quantum communication—or transduction—has been demonstrated and is being actively researched, thereby enabling the concept of a multicore quantum computer.¹³

For computing, there have been large numbers of demonstrations of qubits in a large array of quantum mechanical systems and a plethora of materials systems. Four materials systems: superconducting quantum circuits,^{14–17} semiconductor donor qubits,^{18,19} semiconductor quantum dot qubits,^{20,21} and ion traps^{13,22,23} have been adapted by corporations to develop toward a useful machine. The state of experimental quantum computing has evolved beyond merely searching for

a quantum mechanical system to demonstrate realizations of QIST principles, into advancing hardware implementations that dramatically improve qubit performance and scalability and demonstrations of useful quantum computations.

Materials selection

A significant impact of materials science has been seen in selecting and refining the constituent materials used to make QIST devices. Each technology area has graduated from a Darwinian materials selection process with origins going back decades. While there are indeed vestiges and continued research in designing workaround techniques to leverage a wider range of materials, the leading materials for computational qubits are entrenched, but not finalized.

For spin qubits, nuclear spin-free ($I = 0$) host materials are mandatory for computation and highly desirable for sensing.²⁴ Unfortunately, Group III and Group V elements do not have any $I = 0$ isotopes. Despite manipulation of the nuclear spin bath presented by the host material to minimize its impact,²⁵ there has been a down-selection of optimal materials for QIST. Silicon germanium has replaced gallium arsenide-based materials in quantum computing, while diamond, graphene, and silicon carbide have become favored over gallium nitride and boron nitride in quantum sensing. A few demonstrations of devices made from isotopically enriched materials have proven the impact of eliminating nuclear spins.^{26–29}

The early adoption of two-dimensional electron gases (2DEG) in tensile-strained silicon quantum wells for the basis of silicon germanium qubits has had continued challenges associated with manipulating the conduction-band degeneracy to present a single valley needed for long coherence times.^{30–34} Interestingly, devices such as those shown in **Figure 2** that are fabricated from two-dimensional hole gas (2DHG) in

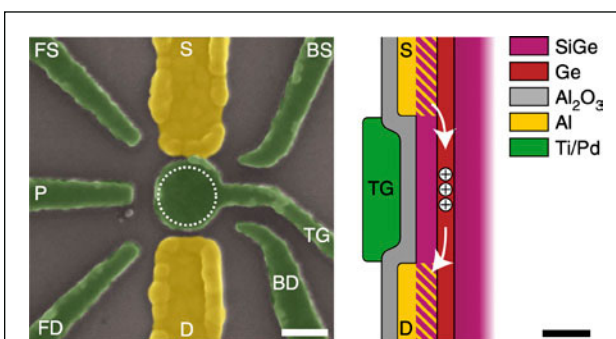


Figure 2. A false-colored scanning electron microscope image of a quantum dot device that is created with holes confined in a compressively strained germanium quantum well into a dot that is defined with the top gate TG (dotted circle). The other electrodes labeled BS, BD, FS, FD, S, D, and P are barrier and finger, source and drain contacts. Along with the central plunger gates, they provide control of the number of holes and energy levels in the quantum. The cross-sectional schematic on the right shows the heterostructure grown using chemical vapor deposition, dielectric layers and metal contacts. Scale bars = 100 nm. Reprinted with permission from Reference 35. © 2018 American Physical Society.

compressively strained germanium are emerging as viable alternatives.³⁵

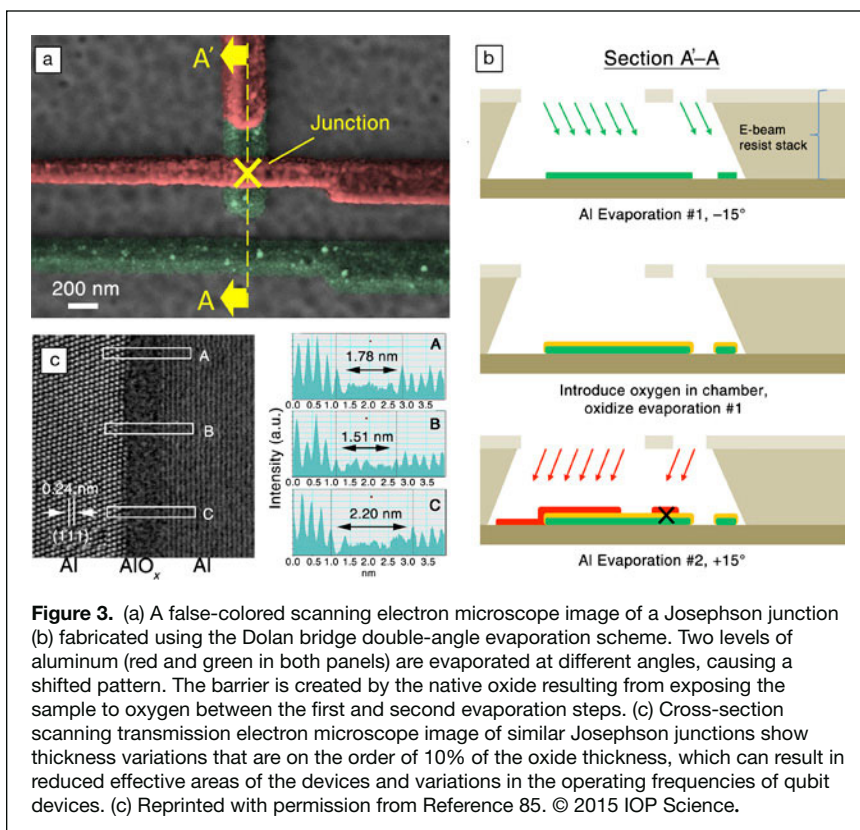
For superconducting qubits, float-zone refined silicon and sapphire have been demonstrated to be extremely useful substrates because of their low microwave loss, while many alternatives (such as MgO) are unsuitable because of their inherent absorption of microwave energy,³⁶ which directly degrades the quantum state lifetime of the qubit. As illustrated in **Figure 3a–b**, superconducting quantum circuits-based Josephson junctions are ubiquitously made from aluminum and oxidized aluminum in the same manner that Giaever constructed his tunnel junctions for his Nobel prize-winning work.³⁷ The drive for a superconductor with a higher critical temperature than aluminum ($T_c \sim 1$ K) is not a research goal in the present context because of the limitations imposed by the DiVincenzo criteria. The penetration and coherence lengths also do not appear to be of primary importance, and a number of superconducting materials have been explored.^{38–40} However, replacing aluminum with a different superconductor that is more robust in fabrication as well as improving circuit-operating tolerances by replacing the Al/AIO_x/Al Josephson junction are likely.

Another major qubit technology is trapped ions, which has evolved toward presumably scalable surface trap geometries⁴¹ that introduce a number of materials challenges associated with the choice of electrode material.²² The community has converged largely on unreactive metals such as gold for the electrode material; however, certain observed universality of behaviors across different metals and demonstrations of state-of-the-art performance with alternative electrode materials^{42,43} keep this an active area of research. Surface cleaning procedures involving ion beams^{44–46} or plasmas⁴⁷ have become commonplace.

Dielectric materials are an important class of materials that are critical in making each of these types of qubits. There are no front runners in terms of the best dielectric, conductor, or optimal deposition techniques to use for surface traps, which offer broad opportunities for new materials to be inserted into qubit devices for both sensing and computing.

Understanding noise from a materials perspective

Overcoming noise is one of the main technical challenges to realize in the next generation of QIST. Practitioners may consider noise from a device perspective and employ labels based on how the noise interacts with the qubit. Without exploring the specific origin, qubits experience charge noise, which is spatial and temporal variation of the electrical



potential, and flux noise, which is spatial and temporal variation of the magnetic vector potential. There are a number of potential sources of these noise types. Some noise sources are “technical,” such as imperfect thermal management, noisy control electronics, and incomplete shielding against remote sources of electromagnetic radiation.⁴⁸ However, perhaps more insidious are noise sources intrinsic to the qubits themselves, originating from the materials used in their fabrication. Such noise sources originate within the sample, where connections to the specific origin may be confined to a precise region, such as an interface between a certain pair of materials,^{49,50} or arise more generally from within the bulk of the sample.

A plethora of possible materials defects and properties that may generate noise within the qubit and contribute to decoherence or unwanted cross-coupling among qubits or quantum states stored within them make optimization of qubit fabrication and materials choices challenging. On the other hand, mitigating the materials origins of noise creates great opportunity for improving their intrinsic performance and enabling across-the-board improvements in the ability to leverage the quantum resources they represent, including enabling greater scalability and/or the ability to implement quantum error correction.

There are a number of engineering strategies that attempt to minimize these effects. Quite often, all of the available concepts are leveraged. These strategies include operational configurations that look toward operational sweet spots that

minimize charge⁵¹ or flux noise effects, designing devices that use energy configurations (i.e., Lambda configuration^{52,53}) that are more stable, and using circuit or cavity quantum electrodynamics.^{54,55} Measurement techniques can also be employed to reduce the impact of some noise, such as Hahn–Echo and Carr–Purcell–Meiboom–Gill (CPMG) sequences. There is also a significant effort to minimize the effects of materials on the qubits. At the cost of circuit density, physically large superconducting circuit elements can be used to move electromagnetic energy away from loss materials (into air or vacuum) in an effort to minimize the interaction between the quantum information and nearby materials.⁵⁶ Some materials are inherently noisy or lossy and are therefore incompatible with certain types of qubits; for example, specific isotopes of certain elements that exhibit non-zero nuclear spin cause inherent decoherence of spin qubits.

Surfaces and interfaces tend to be the location of many sources of noise.^{57,58} Contamination residue and particulates (CRaP) resulting from device fabrication on the nanometer scale at dilute levels is a challenge that has been difficult to quantify.⁵⁹ Once CRaP is mitigated, surfaces and interfaces are inherently challenging because they offer both noise sources from unintended impurities,^{60,61} and under-coordinated bonds⁶² and surfaces that can express a rich variety of energy levels that may produce charge or flux noise.⁶⁰

A rich interdisciplinary area of needed research comprises understanding and identifying the microscopic origins of noise.^{63,64} Some general categories of the origins of such noise have already been identified,⁶⁵ such as two-level system (TLS) defects,^{66–69} quasiparticle loss,^{48,70,71} charge,^{72,73} and flux defects. Qubit devices themselves or similar devices can be used as sensitive sensors to characterize these noises.^{74–77} However, additional understanding of their specific (atomistic) materials origins would be of great value for engineering mitigation strategies. For example, the concept of a TLS defect is an abstraction of the energetics of a class of defects based on their spectroscopic behavior with no connection to atomic or electronic structure. They can interact coherently or incoherently, couple to the qubit, and act as individuals or ensembles.⁷⁸ There have been a few proposed models of microscopic origins, but these calculations have limitations imposed by current computational techniques. Possible origins of charge noise in semiconductors have been conjectured to include a charge particle having an extended wave function, charge hopping among a number of nearly degenerate states, or transport over significant distances on the nanometer scale. However, none of these have been correlated to actual observations or microscopic charge objects. Density functional theory (DFT) suggests that flux noise can arise from adsorbed atoms, magnetic impurities, and metastable bond configurations.⁷⁹ With a few exceptions, most groups producing and measuring qubits are focused on the quantum information aspects, so fewer studies are focused on understanding qubit noise. The limited number of research groups successfully experimenting with qubits results in limited

opportunities currently to correlate qubit function (both good and bad) with detailed characterization of the device, especially with high statistical significance, which requires measurements on a large number of devices.

For materials simulation, the micro-electron-volt (μeV)-scale energy landscape relevant to QIST is challenging for the resolution of most computational techniques, such as DFT. In addition, the large phase space of nearly degenerate atomic configurations complicates the ability to explore experimentally realistic structures and to sample relevant configurations efficiently. Also, large, complex models are often required to represent the relevant details of the materials. Improvements in computational techniques to address these issues of energy resolution, complexity, and system size are needed, as well as access to ever-advancing high-performance computing resources. Clearly, research into computational techniques that are beyond-DFT could provide valuable insights into the microscopic origins of noise in quantum information materials and devices.

Materials synthesis and device fabrication

The reliance of a quantum state to contain information represents an incredible localization that often produces a requirement of atomically precise fabrication. Additionally, the requirement of having a long-lived quantum state dictates that material losses need to be eliminated. While the first generation of QIST devices can accept a low yield, successive generations will need to be reliably made to enable scaled fabrication. The path toward this potential requirement creates a number of challenges in materials synthesis and device fabrication.

For materials synthesis, challenges exist in the growth and integration of novel materials that have not been used in the conventional electronics industry. For starters, intrinsic losses can be circumvented through materials selection, while impurity and defect losses must be addressed through synthesis and fabrication.^{80,81} Therefore, an emphasis has been placed on the synthesis of ultrapure and “perfect” materials, but practically speaking, control and mitigation of the most detrimental defects are generally practiced. Additionally, the localization of the qubit energy is sensitive to decoherence and noise pathways that are often localized to nearby defects and not averaged properties of the host material. The atomic-scale details of materials interfaces and variations in short-range ordering become important.

A particular challenge arises when integration of dissimilar materials is required. Indeed, the interplay between ordered and disordered materials is often critical, for example, in Josephson junctions where disordered insulating materials or oxides are sandwiched between more crystalline metallic layers.^{82–84} As shown in Figure 3c, interface roughness and variations of the dielectric properties on the nanometer scale can greatly affect the tunneling behavior of the Josephson junction because the device characteristics depend exponentially on the effective thickness of the tunnel barrier.^{85–87} It is possible that

new materials systems and epitaxial growth techniques will advance some aspects of QIST devices.⁸⁸

Many QIST devices are fabricated with electron-beam lithography or focused ion beams to achieve the features with critical dimensions below 100 nm. For superconducting qubits, the Josephson junction area has been decreased to be significantly less than $1 \mu\text{m}^2$ in order to reduce the number of defects observed in spectroscopy and decoherence. For semiconductor quantum dot qubits, the confining potential electrodes are on the order of 20 nm. Even diamond nitrogen-vacancy (NV) center quantum sensors have solid immersion lenses,⁸⁹ scanned probes,⁹⁰ and waveguides fabricated⁹¹ at sub-micron scale.

Electron-beam lithography is not the only technique used to pattern important devices at the nanoscale. Scanning tunneling microscopy has been harnessed for lithography and leveraged to create qubit defects from single donor atoms in silicon.⁹² Helium-ion microscopy has also been leveraged to modify materials and create Josephson junctions from high- T_c superconductors.⁹³ Nanoimprint lithography, where a patterned stamp is used to create features, is another emerging technique, and alternative bottom-up strategies of fabrication (so called “advanced additive manufacturing”) are being explored as well,⁹⁴ including approaches for atom-by-atom ultraprecise fabrication and use of layered 2D materials with finite defined thicknesses.⁹⁵

At these length scales, the microstructure impacts feature shape, line edge roughness, and critical dimension control as much as the features of the resist. Improved understanding of plasma interactions with materials for etching, deposition, and cleaning is dramatically impacted by such small patterned features because there is always a sidewall nearby.

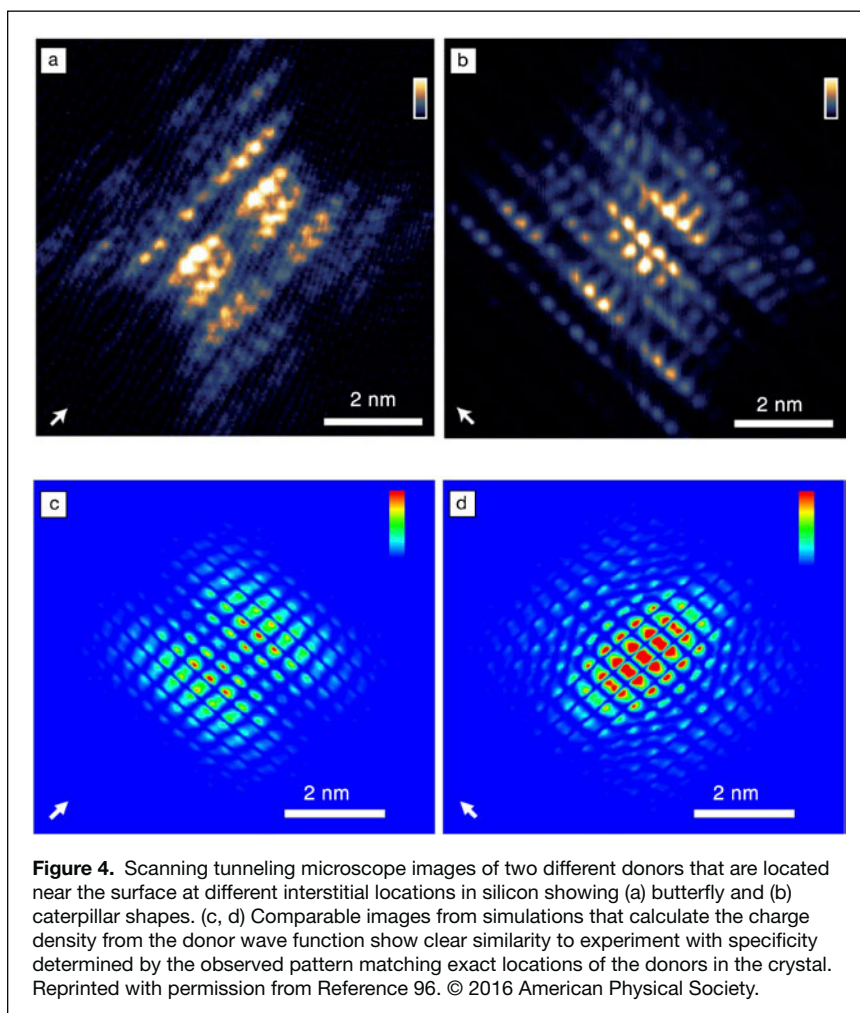
For all of these reasons and more, advancements in materials synthesis, crystal growth, and thin-film process technologies are listed as some of the most desirable contributions needed to advance QIST.

Materials characterization

For measurement science, there is a need to increase the resolution and sensitivity of existing techniques to reach scales relevant to QIST. Structural defects at the atomic scale and electronic energies at the μeV scale affect device performance, but the details of specific defects and their impacts are not well understood.

Perhaps the greatest immediate contribution that applied materials science can make to QIST is in the area of materials characterization. This is because the relatively low yield of devices in academic laboratories and overhead required to produce and test devices has resulted in the physics community relying on just those techniques and materials that work as determined by correlation between specific process recipes of available tools and qubit characterization. Studies using failure analysis techniques and targeted materials analysis correlating material properties with both well-performing and poor-performing bad devices may greatly help in detangling limitations imposed by inherent materials properties from those resulting from materials processing and nano-/microstructure. In this regard, routine characterization of fabrication properties used for yield and failure analysis, borrowed from the microelectronics industry, such as critical dimension and interface roughness, can also play an important role.

The localization and reliance of a single quanta of energy to represent a bit challenges many materials characterization techniques in terms of resolution and sensitivity. That is, there is also a need beyond applied materials science. The fundamental contribution of materials science is needed because



today's qubits operate with characteristic energies that are on the order of $30 \mu\text{eV}$, and our knowledge of materials in this energy regime is sparse. It is worth considering which techniques are at their physical limits and which can be improved through technology improvements such as redesigned stability, collection efficiency, advancements in detector technology, or perhaps data analysis. Our understanding of materials behavior should be sufficient to resolve effects that are energetically comparable or smaller, but only a few materials characterization techniques are capable of this task, and most capabilities of computational materials science are orders of magnitude less accurate and less precise.

Improved imaging and spectroscopic technologies, such as the results highlighted in **Figure 4** that directly investigate quantum wave functions,⁹⁶ have the potential to explore the locality of the quantum information and perhaps gauge interactions with defects and their effects, along with the wider application of existing tools to the field of QIST. This will go a long way toward unraveling the materials impacts of device performance and enable more rational materials selections and device fabrication processes. Advancement and application of a number of analytical techniques will be instrumental. **Figure 5** shows an atomic force microscope using an NV center near the tip apex with fluorescence collected with a confocal microscope. This is one of several emerging quantum probes that may prove essential to such investigations.

Such probes include using color centers (e.g., NV centers) to measure surface magnetic defects, trapped ions as probes of electric field noise, or tuned superconducting or semiconducting qubits as sensitive probes of charge noise.

Another need arises from the expectation that quantum computing devices will continue to operate at cryogenic temperatures. Improving the current understanding of material properties and development of advanced materials with engineered properties at cryogenic temperatures are clear contributions that materials science research can make. Current materials selection at cryogenic temperatures is limited, and much of our knowledge does not extend into the tens of milli-Kelvin temperatures at which qubits operate. Methods of adhesion, coefficients of thermal expansion, thermal and electrical conductivity, and optical/microwave properties, such as dielectric coefficients and loss across the electromagnetic spectrum (particularly in the microwave region of low-temperature thermal photons associated with blackbody radiation), are not well known at cryogenic conditions for many materials currently in use.

The diabolical nature of surfaces and interfaces is experienced by quantum information devices. The negative influence of surfaces has been observed in nearly all qubit technologies for computing and sensing, such as shorter lifetimes and reduced coherence in diamond NV centers, phosphorous donors in silicon, silicon spin qubits, superconductor qubits, and anomalous heating ion trap qubits.^{97,98} As illustrated in **Figure 6**, the microscopic source of anomalous heating such as Johnson noise, surface diffusion of adsorbates, and surface dipole fluctuations have been attempted, but more work is needed to produce significant, reliable, and rational improvements following specific surface treatments and controlled interface contamination.^{44,50,79,99,100} Investment is needed in understanding surface chemistry, passivation, and the connection between atomic configuration and composition to the electronic structure of the surrounding material region on the tens-of-nanometers length scale, with μeV or better energy resolution, and at cryogenic temperatures. Thermodynamic understanding of both stable, metastable, and unstable configurations at energies relevant to the qubit transition energies can have an immediate impact on understanding specific modes of quantum information degradation.

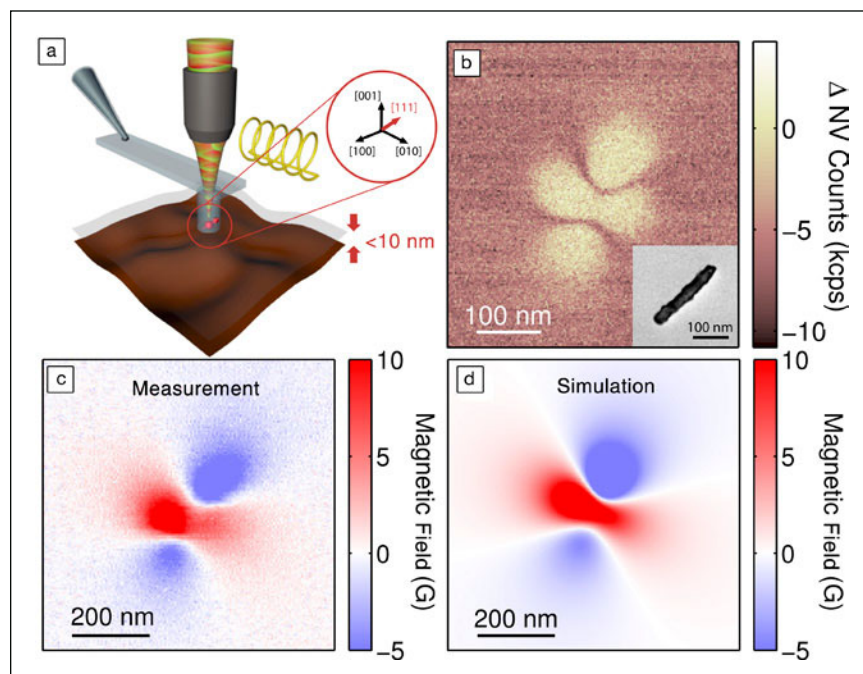


Figure 5. (a) Schematic diagram of the atomic force microscope setup using a nitrogen-vacancy (NV) center near the tip apex with fluorescence collected with a confocal microscope. (b) The measured static-magnetic-field image of a single Ni nanorod, where a negative fluorescence contrast indicates a local field smaller than the detection threshold. The inset shows a scanning electron microscope image of a similar rod. (c) The full field map of a single Ni nanorod compares well with the magnetic field of a point dipole (d) projected onto the NV axis for a NV center located 80 nm above the dipole. Reprinted with permission from Reference 90. © 2016 AIP Publishing.

Emerging engineered materials

Many of the advances in materials science discussed so far fit within the existing framework of demonstrated

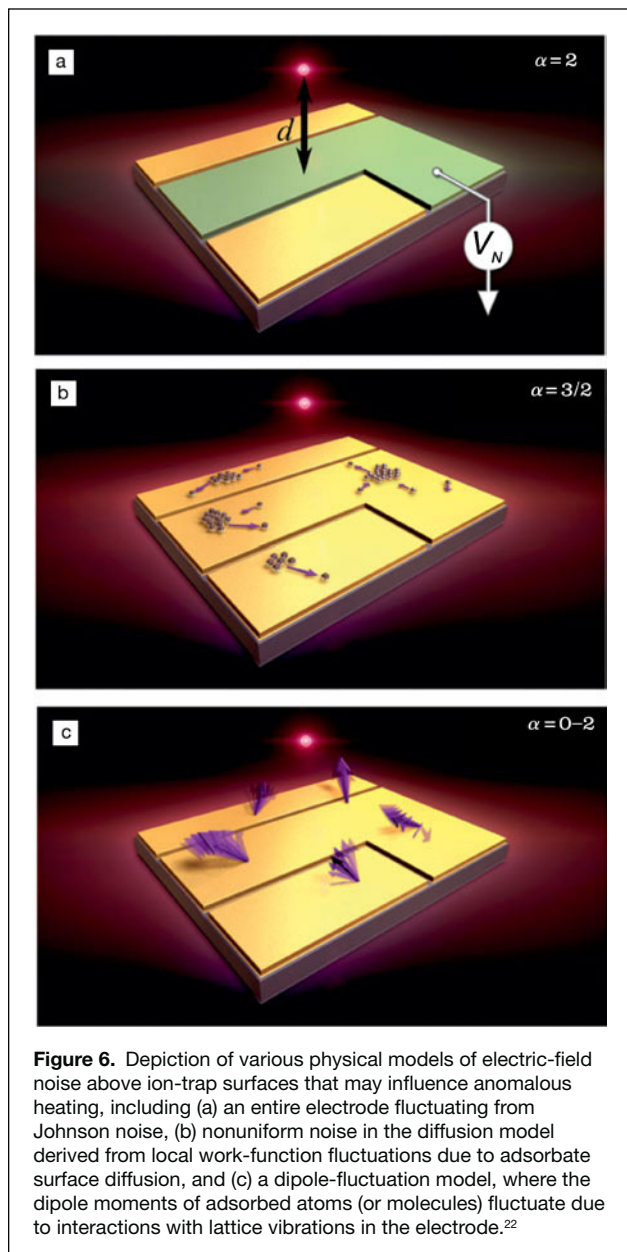


Figure 6. Depiction of various physical models of electric-field noise above ion-trap surfaces that may influence anomalous heating, including (a) an entire electrode fluctuating from Johnson noise, (b) nonuniform noise in the diffusion model derived from local work-function fluctuations due to adsorbate surface diffusion, and (c) a dipole-fluctuation model, where the dipole moments of adsorbed atoms (or molecules) fluctuate due to interactions with lattice vibrations in the electrode.²²

qubits, but there will always be the potential to introduce new qubit materials. QIST is in its infancy, and by analogy is comparable to the pre-integrated circuit technology of digital computers. Nevertheless, if quantum computing follows other technology paths, it is reasonable to expect that this high-risk/reward opportunity may continue to shrink as the existing technologies improve. In addition, different quantum platforms have their own merits, and limitations and successful systems may include hybrid approaches, since it has become clear that no single platform possesses all the advantages, thus interaction between dissimilar qubits is necessary.

Quantum communications may see the first widespread adaption of hybrid systems as data interconnects are required between quantum cores that consist of numerous qubits. Transmission of quantum information is readily demonstrated

in ion trap qubits using optical photons, superconducting qubits using photons coupled through nanomechanical oscillators, and spin qubits directly interacting with photons. Each of these paradigms of quantum transduction in hybrid systems can use advances similar to those already described, and materials innovations from other fields such as integrated optics and microwave engineering can be leveraged.

One example of a near-term hybrid system is the adoption of circuit quantum electrodynamic approaches for spin qubits; another is the use of dispersive readout (a measurement technique used in superconducting qubits) in silicon germanium quantum dot qubits. The integration can also be more intimate, such as voltage-tuned Josephson junctions using a semiconductor element in a superconducting quantum circuit.¹⁰¹ The major challenges are inherent in interfacing any two dissimilar materials (e.g., aluminum and a semiconductor), with different material and electronic properties. As shown in **Figure 7**, current solutions for synthesizing these interfaces include nanowires and innovative configurations to use shadow evaporation to eliminate process contamination. For superconducting devices, losses in or at the interface (with native oxides, dielectrics) could severely limit device performance.^{102,103} In semiconductors, roughness introduces trap centers and charge noise. In these hybrid approaches, it is yet to be seen if the advantages of the constituent systems can be combined to outperform the materials difficulties of them individually.¹⁰⁴

Other types of quantum materials have already evolved into use in quantum information applications. Van der Waals heterostructures made from a variety of 2D materials are actively being pursued as possible Josephson junction materials, and topological materials may also find use in qubit devices.^{105–107} Other types of quantum materials may enable a whole new class of qubit devices. Topological Majorana zero-mode (MZM)

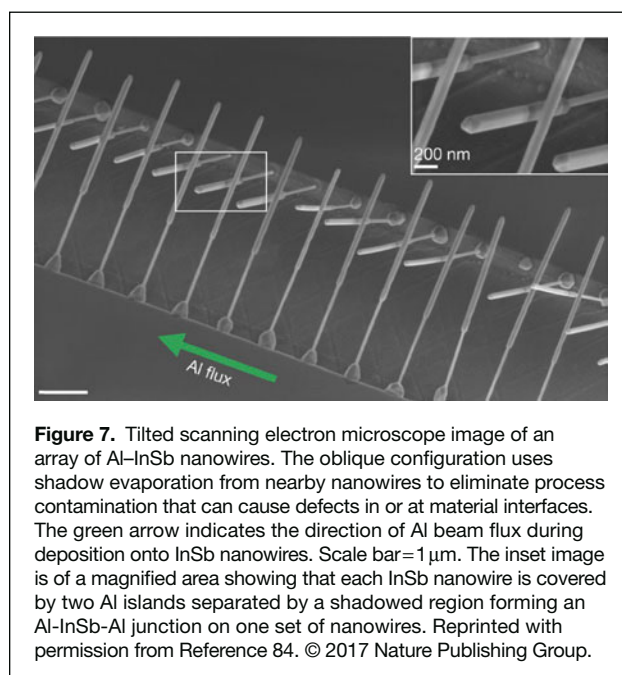


Figure 7. Tilted scanning electron microscope image of an array of Al-InSb nanowires. The oblique configuration uses shadow evaporation from nearby nanowires to eliminate process contamination that can cause defects in or at material interfaces. The green arrow indicates the direction of Al beam flux during deposition onto InSb nanowires. Scale bar = 1 μm . The inset image is of a magnified area showing that each InSb nanowire is covered by two Al islands separated by a shadowed region forming an Al-InSb-Al junction on one set of nanowires. Reprinted with permission from Reference 84. © 2017 Nature Publishing Group.

qubits have received significant interest and investment in the hope of providing inherent topological protection against noise/decoherence. Topological qubits are postulated to provide intrinsic fault-tolerant computation at the hardware level, which, in principle, should drastically reduce the overhead associated with fault-tolerant quantum computing, which otherwise requires a significant multiplication of qubit count.^{108–115} MZMs possess non-Abelian exchange statistics similar to exotic quantum Hall states with non-Abelian statistics. Topologically protected operation can be carried out by exchanging the MZMs on the circuit, yielding the nontrivial transformation that may be used to implement some quantum gates.¹¹⁶ MZM devices are a fascinating area of research that combine semiconductors, normal metals, and superconductors; but there are a number of real material challenges in creating and observing them.

Topological superconductivity relies on synthesis of new material combinations, combining superconductivity, low density, and spin-orbit coupling.^{117–119} Since the MZM is formed at the interface between the superconductor and the semiconductor, the epitaxial growth of superconductors on semiconductors with strong spin-orbit coupling has received renewed attention. Epitaxial growth of Al on InAs nanowires and heterostructures containing 2DEGs near the surface have been shown to yield a high-quality superconductor-semiconductor system with uniformly transparent interfaces¹²⁰ and a hard-induced gap, indicated by strongly suppressed subgap tunneling conductance. It is possible that the technological impact of topological protected states is reduced if MZM qubits are not developed at the rate of or faster than other qubit systems, since traditional quantum error correction approaches using surface codes based on stabilizers on a two-dimensional array¹²¹ and other logical qubit configurations can provide comparable benefits from a wider range of qubit implementations.

Quantum sensing is at an exciting time. The value of spin-based quantum sensing using defects in diamond has shown great promise. While most work has been completed with the well-known NV center, other defect complexes such as silicon vacancies, germanium vacancies, and perhaps tin-vacancies in diamond offer a range of properties that are important to sensing applications. Additionally, new materials such as silicon-vacancies in silicon carbide and defects in boron nitride and gallium nitride offer other avenues for different sensors to be engineered.

Critical non-qubit materials technologies

A number of auxiliary technologies for QIST can also benefit from materials advancements. Some examples include surface traps with integrated photonics for ion traps,¹²² 3D superconducting circuit integration,¹²³ superconducting ribbon cabling for both controlled thermal and electrical transport.^{124,125} Functional coatings and adhesives that can withstand dramatic differences in thermal expansion coefficients could benefit all qubits that operate at millikelvin temperatures.¹²⁶ Furthermore, the materials advancements for improved qubits can be leveraged for improved quantum sensors and communications devices, as outlined previously.

Outlook

Quantum information science is an interdisciplinary technology, with materials science having a clear and important role to play. For solid-state qubits, materials synthesis and device physics will undoubtedly play a major role in advancing the state-of-the-art technology. Research contributions are possible from individuals in all types of organizations. Academic labs that focus on individual and pairs of qubits, emerging qubit materials, and fundamental correlations between materials and qubit performance will continue to provide value to the maturing QIST community by training its workforce and exploring innovations that may lead to disruptive technologies. Improving fundamental behavior and understanding qubit material interactions should advance all aspects of QIST. It is expected that fast-paced interactive collaborations among research groups that span specializations will become more common, and materials scientists who understand the requirements of QIST will be in high demand.

The pathway to commercial relevance in quantum sensing is not as steep as quantum computing. The current landscape of startups, established corporations, and academic groups all contributing to advancing the state of the art of quantum sensing is likely to be sustainable.

Corporations have already moved into quantum computing and will most likely dominate systems development and technology demonstrations in the upcoming “noisy intermediate-scale quantum” (NISQ) computing era.¹²⁷ The field has seen hiring and growth, and academia can contribute by producing a trained workforce that is skilled in traditional areas in addition to training in modern physics such that graduating students can compete in the quantum workforce. It is not clear what materials and design will move QIST beyond NISQ, nor is it clear how long this will take, but materials science will continue to be a critical aspect of this technology moving forward.

Improvements in high-throughput fabrication and device testing would allow better statistics to be collected that correlate device performance with fabrication conditions, so that fabrication-related artifacts can be distinguished from intrinsic limitations of the constituent materials and fabrication tolerances improved. The state-of-the-art in QIST should be compared to the knowledge base for conventional electronics processing and fabrication, where enormous amounts of data enabled by the well-established fabrication infrastructure drive very targeted and controlled fabrication processes informed by well-understood correlations between process and device function. As centers focused on quantum information science and technologies emerge, it is important that materials scientists participate in the community and contribute to quantum technologies as we have done in many traditional technologies.

Summary

Materials science has a central role in the emerging quantum information technology industry. Both applied and fundamental opportunities in the field provide a range of

contributions that materials scientists can make in a variety of materials systems, including superconductors, semiconductors, insulators in thin films, and bulk. Surfaces and interfaces are important, particularly between dissimilar materials. Perhaps the largest contribution that materials researchers can make is to enhance our understanding of materials at cryogenic temperatures with energy resolution on the μeV scale.

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