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Quantum Grover search-based optimization for innovative material discovery

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***Abstract*—Advances in data analysis, machine learning, and combinatorial optimization have accelerated the discovery of new materials with desired properties; this paradigm is commonly referred to as Materials 4.0. Quantum computing represents a new computing framework that uses the principles of quantum mechanics such as entanglement and superposition. Quantum algorithms such as Grover search has been proven to have quadratic speedup over the classical search methods. This paper considers the application of Grover search-based combinatorial optimization for material discovery. In particular, this paper considers the identification of the Nickel-Titanium (Ni-Ti) based shape memory alloy of the composition, $Ti_{50}Ni_{50-x-y}Cu_xFe_y$ that has the minimum thermal hysteresis associated with the austenite-martensite transformations. The paper details the construction of quantum circuits to carry out the optimization analysis, and demonstrates the analysis on a simulation platform using the Python Qiskit package.**

***Index Terms*—Quantum, Grover, Material, Discovery, Data, Shape Memory, Optimization**

I. Introduction

Discovery of high performance and functional materials can often lead to significant technological benefits such as development of energy-efficient sustainable systems, lightweight, and high strength structural systems. Traditional methods for material discovery such as experimental techniques, theoretical methods, and simulations are often time-consuming and/or computationally expensive. Recent advances in data collection, data storage, and data analytics in the domain of material science has led to a new data-driven paradigm for material discovery known as Materials 4.0 [1].

Iyer et al [2] used a Bayesian optimization framework where stochastic models such as Gaussian process (GP) models are used to build relationships between the material compositions and target material properties; these models are then used in the material discovery process. Several types of data-driven models such as artificial neural networks (ANN), supper vector regression (SVR), and relevance vector machines (RVM) have also been used to build quantitative relationships between material compositions and properties [3]. Mannodi-Kanakkithodi et al [4] used kernel ridge regression for data-driven modeling and genetic algorithms for accelerated design of polymer dielectrics. Gopakumar et al [5] used GP and SVR models along with multi-objective formulation to discover material designs with desired properties. The multi-objective optimization results were represented using a Pareto surface, which was used for identifying the optimum material design.

Data-driven techniques coupled with the availability of high-performance computing systems have greatly reduced the material discovery time. With the recent advancements in quantum machine learning and computing, the discovery time can further be reduced by implementing quantum algorithms for optimization analysis. Quantum computing represents a new paradigm of computing that uses the properties of quantum mechanical systems such as entanglement and superposition [6]. Quantum algorithms such as Grover search and Shor's algorithm have theoretically been proved to surpass the classical algorithms in computational complexity [6]. In this paper, we seek to leverage the computational benefits of quantum Grover search algorithm [7] for accelerated material discovery. In particular, we consider the discovery of Nickel-Titanium (NiTi) based shape memory alloy (SMA) that minimized the thermal hysteresis. The thermal hysteresis can be directly related to the functional fatigue characteristics of SMAs. Therefore, discovering material compositions with small thermal hysteresis can reduce the functional fatigue in SMAs, which increases the material's functional stability [8].

The rest of the paper is organized as follows. Section II provides a brief background to quantum computing, Grover search, and Grover search-based optimization. Section III details the quantum circuits that facilitate Grover optimization. Section IV details Grover optimization for discovery of NiTi-based SMA, and Section V provides the concluding remarks.

II. Background

A. Qubit

A qubit is elementary representation of information in quantum computing. As opposed to a classical bit, a qubit is in both 0 and 1 states simultaneously; this phenomenon is referred to as quantum superposition. When a measurement is made on the qubit, it chooses one of the two states: 0 or 1. The Bra-Ket notation is commonly used to represent a qubit as $|\Psi\rangle = a_1|0\rangle + a_2|1\rangle$, where $|\Psi\rangle$ denotes the superposition state, and $|0\rangle$ and $|1\rangle$ represent the basis states [9]. a_1 and a_2 are the probability amplitudes that correspond to the behavior of the qubit. The probability amplitudes can be complex numbers and belong to $\mathbb{C}$ space. Given the probability

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amplitudes, the probabilities that the qubit chooses $|0\rangle$ and $|1\rangle$ states upon measurement are given as $\bar{a}_1 a_1$ and $\bar{a}_2 a_2$, where $\bar{a}_1$ and $\bar{a}_2$ are complex conjugates of a_1 and a_2 respectively. When multiple qubits are used in computing, their joint state can be obtained through a tensor combination of individual qubits. If $|\Psi_1\rangle$ and $|\Psi_2\rangle$ represent two qubits, then their joint state is $|\Psi_1\rangle \otimes |\Psi_2\rangle$. Another important property of quantum systems is quantum entanglement, which corresponds to interactions between individual qubits. A set of entangled qubits cannot be mathematically described as tensor product of individual qubits. The entanglement property is used to encode the dependence between individual qubits.

B. Qubit transformations

Similar to the use of gates in classical computing for bit transformations, quantum gates are used for qubit transformations. There are several elementary gates that act on a single qubit, two qubits, and three qubits. Any other complex multi-qubit transformations can be decomposed using these elementary gates. We discuss some of the gates that are later used in optimization analysis for material discovery.

1) One qubit gates: With respect to one qubit gates, we will discuss the X, H, and Z gates. The X gate (also known as Pauli-X gate) flips the $|0\rangle$ to $|1\rangle$ and vice versa. The Hadamard gate or the H gate creates equal superposition of $|0\rangle$ and $|1\rangle$ states, but with different amplitudes, when acting on $|0\rangle$ or $|1\rangle$ basis state. The Z (also called the Pauli-Z gate) does not have any effect on $|0\rangle$ state but changes the sign of the probability amplitude corresponding to $|1\rangle$ state.

2) Two qubit gate: With respect to the two qubit gates, we discuss the CZ gate (or the Controlled-Z gate). The two qubits on which the CZ gate acts on are referred to as the control qubit and the target qubit. When the control qubit is $|0\rangle$, then there is no effect on the target qubit whereas when the control qubit is $|1\rangle$, then the Z gate acts on the target qubit.

3) Three qubit gate: Among the several available three qubit gates, we will discuss the CCX gate (also called the $CCNOT$ gate and the Toffoli gate). In this gate, two qubits are control qubits, and the third is the target qubit. When both the control qubits are in $|1\rangle$ state, then the X gate is implemented on the third qubit. More details regarding various one, two, and three qubit gates are available in [9].

C. Grover search

After discussing the fundamentals of quantum computing, we now discuss the Grover search algorithm, one of the foremost quantum algorithms that demonstrated the computational superiority over comparative classical algorithms [7]. Grover search is used to search a database of randomly ordered inputs to identify a particular input that corresponds to a desired output. When there are N entries in the database, the classical algorithms have a computational complexity of $\mathcal{O}(N)$, whereas the Grover's search has a complexity of $\mathcal{O}(\sqrt{N})$, providing a quadratic improvement. Let the N entries be represented by a system of n qubits. Let $\mathbf{x}$ represent the vector of all inputs, and $\mathrm{x} = \mathrm{x}_o$ represent the desired input. Let the output at $\mathrm{x} = \mathrm{x}_o$ be denoted as $f(\mathrm{x} = \mathrm{x}_o) = 1$, and $f(\mathrm{x}) = 0$ when $\mathrm{x} \neq \mathrm{x}_o$ .The analysis steps are given below.

1) Create an equal superposition of all the states using the H gates; $|0\rangle^{\otimes n} \rightarrow H^{\otimes n}|0^n\rangle$.
2) Apply a gate (O) defined as $O|\mathbf{x}\rangle = (-1)^{f(\mathbf{x})}|\mathbf{x}\rangle$. This transformation is commonly known as the oracle. The oracle flips the sign of the probability amplitude associated with the desired input.
3) Apply another gate (R) defined as $R|\mathbf{x}\rangle = H^{\otimes n}(2|0^n\rangle\langle 0^n| - \mathcal{I}_n)H^{\otimes n}|\mathbf{x}\rangle$. This amplifies the magnitude of the probability amplitude of the desired input and reduces those of the non-desired states.

One analysis of steps 2 and 3 is considered as one Grover rotation. When $\frac{\pi}{4}\sqrt{N}$ Grover rotations are performed, and a measurement is made on the system, then the probability of observing the desired input is maximized. Please refer to [7] for more details about the algorithm.

D. Grover search-based optimization

The key idea in Grover search-based optimization (also referred to as Grover optimization) is to perform multiple iterative Grover search analyses with varying thresholds.

Since the number of desired inputs for a given threshold is unknown, the number of Grover rotations to be performed is also unknown. Note that $\frac{\pi}{4}\sqrt{N}$ is the optimum number of Grover rotations when only first desired state is present. Several heuristic-based algorithms were developed in the literature to identify the optimal Grover rotations for Grover optimization. We use the Durr and Hoyer as corrected by Baritompa et al (DHB) [10] algorithm in the paper for Grover optimization. A brief introduction to the algorithm is given below. Let $\mathbf{x}$ represent the set of all the available inputs. λ, the algorithm parameter is assumed to be equal to 1.34 (as suggested in [10]).

1) Set the algorithm parameter m equal to 1. Let t represent the threshold value in the current iteration of analysis.
2) Compute the number of Grover rotations to performed (r) by randomly selecting a integer such that $0 \leq r < m$
3) Perform Grover search analysis with r Grover rotations and make a measurement on the system ($\mathrm{x} = \mathrm{x}^*$), and compute its function value ($f^* = f(\mathrm{x}^*)$).
4) If $f^* < t$, then $t = f^*$ in the next iteration, else the threshold value remains the same in the next iteration but $m = \lambda m$. Steps 2,3, and 4 are repeated until the global optimum is obtained.

III. Quantum Circuit

Here, we detail the construction of a quantum circuit to realize Grover optimization, which uses Grover search. We illustrate the construction process using a 3-qubit system, which can represent $8(= 2^3)$ different states. Fig. 1 provides an schematic quantum circuit of Grover search. H represents the Hadamard gate, and O and R represent the Oracle and Reflection transformations as detailed in Steps 1,2, and 3 of Section II. C. After carrying out the various steps, a measurement is made on the system ('meter'symbol).

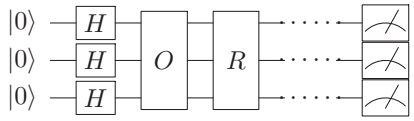
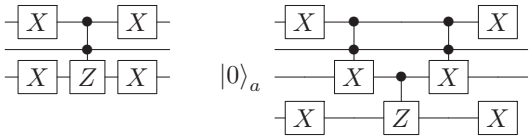


Fig. 1: Illustrative quantum circuit of Grover search analysis



(a) Original (b) Using ancilla qubit

Fig. 2: Oracle corresponding to state $|010\rangle$

The oracle transformation has a different set of gates for different desired inputs (quantum states). The oracle transformation corresponding to state $|010\rangle$ is given in Fig. 2(a). Since CCZ is not an elementary gate, it is decomposed in a set of elementary gates using an ancilla qubit [9] as shown in Fig. 2(b). Ancilla qubits are additional qubits that are used to carry out the required transformation on a given set of qubits. Consider a threshold value in a given Grover optimization iteration that results in two desired inputs, whose function values are less than the threshold value. In such a case, an oracle can be obtained by placing oracles corresponding to each desired input sequentially. Fig. 3 provides the oracle that corresponds to two states $|010\rangle$ and $|000\rangle$, whose function values are less than the defined threshold. This oracle is obtained by stacking the oracle that corresponds to $|000\rangle$ in series with the oracle that corresponds to $|010\rangle$ (Fig. 2(b)).

Fig. 4 provides the quantum gates that are required to perform the reflection transformation. Fig. 4(a) provides the original transformation, which contains a non-elementary CCZ gate, and Fig. 4(b) performs the reflection transformation using the ancilla qubit (similar to the oracle transformation in Fig. 2(b)). Thus, the quantum circuit for the Grover search

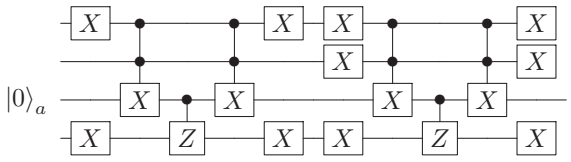
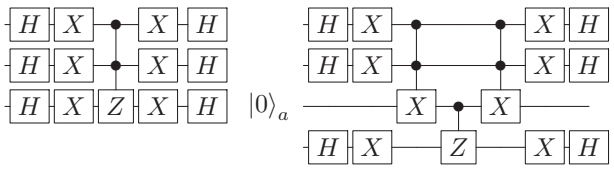


Fig. 3: Oracle corresponding to two states $|010\rangle$ and $|000\rangle$



(a) Original (b) Using ancilla qubit

Fig. 4: Quantum gates for reflection transformation

and optimization can be composed using the quantum gates associated with the Hadamard, oracle and reflection transformations. In the case of an n-qubit system, we are required to carry out the $C^{n-1}Z$ transformation (n-1 control qubits); this is implemented using an additional $n-2$ ancilla qubits. Therefore, the total number of qubits required in the analysis are $n+n-2=2n-2$. When $n=3$, $2n-2=4$ as observed in Figs. 2(b) and 4(b). More details regarding ancilla qubits to perform $C^{n-1}Z$ transformations are available in [9].

IV. NiTi-based shape memory alloy discovery

In this section, we discuss the application of Grover search-based optimization for discovery of a Nickel-Titanium (Ni-Ti) based alloy composition of the form $Ti_{50}Ni_{50-x-y}Cu_xFe_y$ with the minimum thermal hysteresis, where x and y represent the percentage compositions of copper (Cu) and iron (Fe) respectively. We constrain the maximum values of x and y to 5, i.e., $0 \leq x \leq 5$ and $0 \leq y \leq 5$. We use a dataset between the various NiTi-based material alloy compositions of the form $Ti_{50}Ni_{50-x-y-z}Cu_xFe_yPd_z$ and the thermal hysteresis values obtained from Xue et al [11]. This dataset contains 57 data points, and we use this dataset to train a neural network model between the material composition and the thermal hysteresis. We use this neural network model to identify the optimum $Ti_{50}Ni_{50-x-y}Cu_xFe_y$ composition, after fixing the proportion of palladium (Pd) to zero. Following Section II.C and II. D, the neural network model is used in the construction of the oracle given a threshold value. For illustration, we considered x and y in the increments of 0.5 and 0.25 respectively. Since x and y lie between 0 and 5, we have 11 values of x, and 17 values of y, resulting in a total of 187 alloy compositions (11×17).

The number of qubits required to represent these 187 compositions is n = $\lceil \log_2 187 \rceil$ = 8, where $\lceil . \rceil$ represents the ceiling function. When the number of qubit states is greater than the available material configurations, the remaining quantum states are mapped to 'dummy'material configurations. Since the number of required qubits (n) is equal to 8, the number of ancilla qubits required to implement Grover rotation is equal to 6, totaling to 14 qubits. The circuit construction and the optimization analysis are performed using Qiskit, a Python package for quantum computing simulations [12].

The minimum thermal hysteresis value from the dataset is 2.72. Hence, the global minimum of the thermal hysteresis should be less than or equal to 2.72. Given this information, we have two strategies for choosing the initial threshold value: (1) Choose the minimum value from the dataset, i.e. 2.72; and (2) Choose a value that is lower than the minimum value from the dataset (2.72) and perform the optimization analysis. If the analysis does not output any solution, i.e. there is no material composition that has a thermal hysteresis value lower than the threshold, we increase the threshold to a value greater than the previous threshold but less than 2.72. A drawback with the first approach is that when there are several material compositions whose thermal hysteresis values are less than 2.72, then the complexity of the quantum circuit (number of gates) increases.

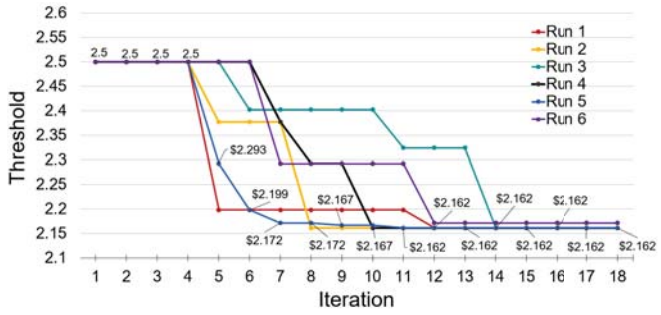


Fig. 5: Convergence of the optimum thermal hysteresis values

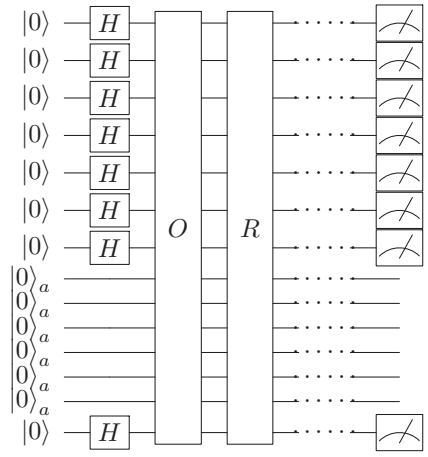


Fig. 6: Schematic quantum circuit of an 8-qubit system with 6 ancilla qubits for Grover search-based optimization

By choosing a value less than 2.72 as our initial threshold, we can reduce the complexity of the quantum circuit.

In this paper, we illustrate the second approach, and consider 2.5 as the initial threshold. Fig. 6 details the quantum circuit with 8 qubits to represent the 187 material compositions and an additional 6 ancilla qubits, to represent the C^7Z gate needed for representing the oracle and the reflection transformations, as detailed in Figs. 2 and 4. The number of Grover rotations that need to be performed is obtained by the DHB algorithm steps as discussed in Section II. D. For a given threshold, if h Grover rotations are required, then the quantum circuit can be represented as $H - O - R - O - R...O - R - M$ where the oracle and reflection transformations are repeated h times followed by a measurement (M), and H represents the Hadamard transformation on the 8 qubits as shown in Fig. 6. The measurements are taken only on the qubits used to represent the material compositions and not the ancilla qubits.

The optimization analysis was carried out using the DHB algorithm discussed in Section II. D. Due to the stochastic nature of the quantum systems, the variation of the threshold values with iterations changes. Hence, we performed the optimization analysis six times, and Fig. 5 shows the variation of threshold values with iterations in the six optimization runs.

The number of material compositions whose thermal hysteresis values is less than the initial threshold is 10. Following Section III, we constructed an oracle for each of the 10 states individually, and placed them sequentially (similar to Fig. 3) to obtain the overall oracle. As the threshold value decreases, the number of desired quantum states decreases; therefore, the complexity of the oracle also decreases.

V. Conclusion

This paper illustrated the application of Quantum Grover search-based optimization for innovative material discovery. Quantum Grover search algorithm was proven to have a superior computational performance compared to classical algorithms for search analysis. Material discovery is one of the scientific domains that can theoretically benefit from the computational benefits of quantum computing. This paper demonstrated Grover optimization analysis for discovery of a Nickel-Titanium (NiTi) based shape memory alloy (SMA) of the composition $Ti_{50}Ni_{50-x-y}Cu_xFe_y$ that possesses minimum thermal hysteresis. Shape memory alloys are commonly used as actuators in several mechanical systems, and identification of smaller thermal hysteresis SMA improves their functional stability and results in increased performance. Qiskit, a python package for quantum computing simulations is used to perform the optimization analysis. Future work should consider illustration of Grover search-based optimization for problems with a large number of possible material configurations. Moreover, future work should also consider implementing the optimization analysis on real quantum computers (such as IBM Q).

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