Quantum Algorithm for Multislice Method

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In recent years there has been a dramatic increasing interest in quantum computing, which offers the promise of gaining significant speedup and solving certain problems that are intractable for classical computing. It is worth studying how to apply quantum computing to practical physical simulation. In this work, we present a quantum algorithm of multislice method based on quantum circuit model to simulate electron wave function propagation and diffraction in thick crystalline specimens. Multislice method [1] is widely used to simulate the elastic interaction of an electron beam with matter in electron microscopy. It can handle complex nonperiodic potential field better than other methods such as Bloch wave method, but for the classical algorithm, the computation cost increases fast as the size of the simulated object increases. We replace the core of classical multislice method by a quantum version to gain advantages in time complexity and storage memory requirement over the classical algorithm, taking advantage of the feature of quantum computing. Most importantly, we replace classical fast Fourier transform (FFT), which is the most time-consuming part of the classical algorithm, to quantum Fourier transform (QFT) [2], gaining an exponential speedup. Furthermore, with the size N of the system increasing, comparing with O(N) bits that are needed for the classical algorithm, we only need O(log$N$) qubits for the quantum algorithm by taking advantage of entanglement of qubits.

The rest parts of the multislice method are also reconstructed accordingly using quantum circuit, which are mainly parts for the phase operations corresponding to the momentum operator and the potential operator. In order to optimize these parts further and construct more efficient quantum circuits, we introduce Walsh transform to decompose these operators to take full advantage of quantum computing [3]. In this way, we can simplify the quantum circuit to execute the operator accurately with fewer quantum gates. We can also decrease the number of quantum gates further within a given error tolerance by selectively ignoring some certain terms with relatively small coefficients after the Walsh transform.

To verify the feasibility of the quantum algorithm, we have simulated quantum circuit on classical computer to implement the quantum algorithm. We use basic plane wave as incident electron wave and successfully obtained the simulation results of electron density distribution and electron diffraction pattern for Au crystal as shown respectively in Figs. 1 & 2 for example, which completely agree with those obtained by classical algorithm of multislice method. Other forms of incident wave are also proved to be useable. We have also investigated the complexity of the quantum algorithm quantitatively. We count the number of quantum gates used in our quantum algorithm for the evolution of one slice, and compare it with the number

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of unit operations of the classical algorithm. The result comes that the quantum algorithm requires fewer logic gates than the classical algorithm as the simulating scale increasing. This work may indicate the possibility of applying quantum computing to electron wave function simulation and achieving quantum advantage in this method.

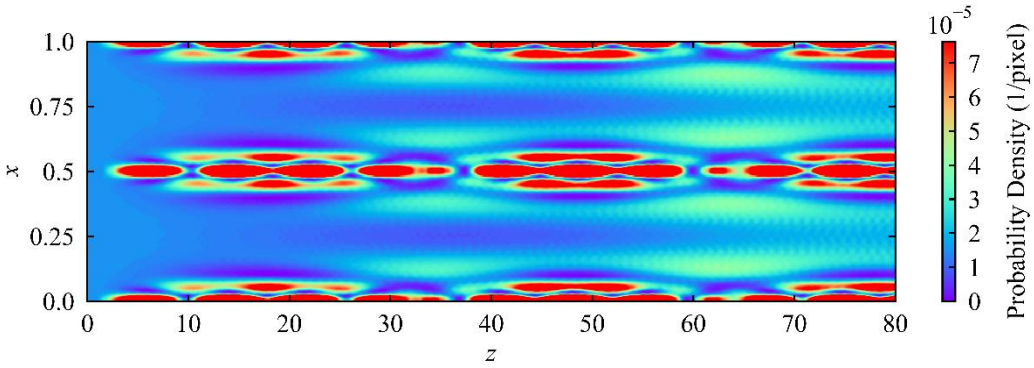

Figure 1. Cross sectional view of electron density distribution in Au crystal, using lattice constant as the unit length. The electron beam is in z axis direction.

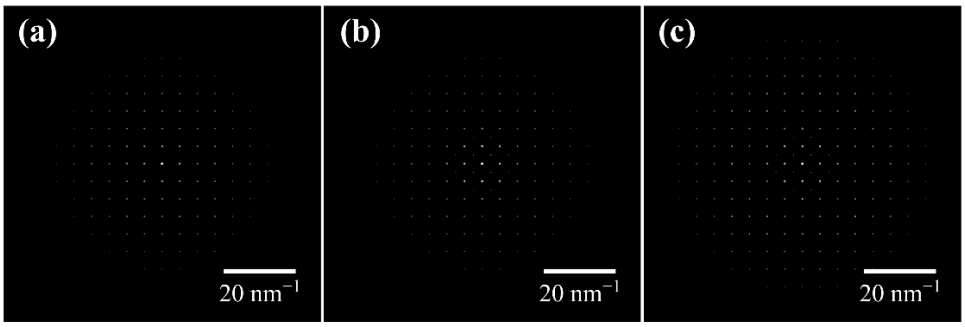

Figure 2. Electron diffraction patterns of Au crystal at different depths.

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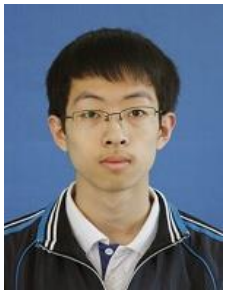
BIOGRAPHY



Y.C. Wang has completed his Bachelor degree in 2018 at University of Science and Technology of China. Now he is pursuing PhD under supervision of Prof. Z.J. Ding.