Novel Quantum Trajectory Approaches to Simulation of Electron Backscatter Diffraction

Long Cheng, Z. J. Ding

Hefei National Laboratory for Physical Sciences at the Microscale and Department of Physics, University of Science and Technology of China, Hefei, Anhui 230026, People’s Republic of China

† Corresponding author: zjding@ustc.edu.cn

Received: 12 December, 2019, Accepted 24 March, 2020, Published 4 April, 2020

We present two quantum trajectory approaches for the simulation of electron backscatter diffraction (EBSD). The quantum trajectory approaches are based on Schrödinger equation and they yield excellent agreements with experimental patterns. Meanwhile, they are particle models that allow ones to intuitively understand the processes of electron diffraction in a classical way. Besides, the approaches have significant advantages in computation efficiency. Because of the accuracy, intuitiveness, and efficiency, the trajectory approaches allow us a deeper understanding of the physical processes of EBSD.

Keywords Bohmian mechanics; EBSD; Quantum trajectory; Electron microscopy

I. INTRODUCTION

Electron backscatter diffraction (EBSD) [1] is a scanning electron microscope (SEM) [2] based technique for microstructure investigation, which provides us important material information for grain boundary characterization and phase identification. Such information is helpful for designing material properties and microstructures. EBSD has certain benefits in microstructure characterization, including simple sample preparation, the high speed of data collection and the high spatial resolution (tens of nanometers). Thus, in the past two decades, EBSD has been widely employed in the researches of metals, alloys, ceramics, semiconductors, and superconductors.

An EBSD pattern consists of characteristic Kikuchi bands, which are a series of parallel bright bands formed by electron diffraction on crystal planes. Kikuchi pattern was first observed by Kikuchi and Nishikawa in 1928 [3, 4], and it has attracted much research interest that how the characteristic Kikuchi bands are formed. First, in the geometric model, Kikuchi bands seen on the screen are gnomonic projections of a set of diffracted cones [5]. Those cones are formed by Bragg reflection and appear in pairs, which make the edges of Kikuchi bands hyperbolic. The geometric model successfully explains the contour of Kikuchi bands, however, it could not explain the observed intensity. Then a dynamic model was developed by Reimer [2] and extended by Winkelmann [6]. It can exactly describe the intensity distribution of Kikuchi bands from the perspective of the wave function.

The dynamic model generally explains the backscattering of electrons in a crystal by calculating the depth integral of probability density [7, 8]. Nevertheless, it cannot intuitively reproduce the processes that how electrons move in a crystal under interaction with crystal potential in a classical picture, and how diffraction patterns are formed and contributed by many single electrons. For the purpose of extracting the maximum amount of crystallographic information from an experimental EBSD pattern, it is necessary to simulate the physical processes of the formation of characteristic Kikuchi bands.

In this work, we start with the fundamental property of electrons, namely the wave-particle duality, and present two quantum trajectory approaches for the simulation of EBSD: i.e., Bohmian mechanics (BM) method and momentum expectation (ME) method. The quantum trajectory approaches are based on Schrödinger equation and they can yield excellent agreements with both the geometrical
structure and the intensities of an experimental EBSD pattern. Meanwhile, they are particle models that allow ones to intuitively understand the process of electron diffraction in a classical way. In other words, the quantum trajectory approaches take into account both the particle nature and the wave nature of electrons, so that they enable us a better understanding of electron diffraction in crystal lattices.

II. METHOD

The main idea of quantum trajectory methods is to associate the particle nature of the electron with the wave nature, that is, an electron is a particle guided by a wave function. Here we have two alternative approaches, namely the BM approach and the ME approach.

A. Bohmian mechanics method

As early as 1925, de Broglie had proposed the concept of the pilot wave, a particle interpretation hypothesis of quantum mechanics [9]. Later in 1952, Bohn developed it into a hidden variable theory of quantum mechanics, thereby establishing the Bohmian mechanics [10, 11].

The Bohmian mechanics begins with the Schrödinger equation,

\[ i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V(r) \psi. \]  

(1)

The wave function \( \psi \) is a complex function, which can be expressed in the polar form,

\[ \psi = R \exp \left( \frac{iS}{\hbar} \right), \]

(2)

where \( R \) and \( S \) are the amplitude and the phase of wave function, respectively. By separating the real and imaginary parts of the Schrödinger equation, we can get the following formulas [12, 13],

\[ \frac{\partial S}{\partial t} + \left[ \frac{(VS)^2}{2m} + V(r) - \frac{\hbar^2}{2m} \frac{\nabla^2 R}{R} \right] = 0; \]

(3)

\[ \frac{\partial R^2}{\partial t} + \nabla \cdot \left( \frac{R^2 \nabla S}{m} \right) = 0. \]

(4)

Equation (3) is a quantum Hamilton-Jacobi equation, which is similar to a classical Hamilton-Jacobi equation, \( \partial S/\partial t + p^2/2m + V(r) = 0 \). In the square bracket in Eq. (3), \( (VS)^2/2m \), \( V(r) \), and \( -(\hbar^2/2m)/(\nabla^2 R/R) \) are the kinetic energy, the classical potential energy, and the quantum potential energy, respectively. So, in Bohmian mechanics, \( VS \) is interpreted as a momentum, \( p \). Thereby, Eq. (4) is just a continuity equation,

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0, \]

(5)

where \( \rho = \psi \psi^* = R^2 \) and \( \mathbf{v} = p/m = \nabla S/m \).

Bohmian mechanics gives another interpretation of the Schrödinger equation. Trajectories of photons [14], electrons, etc. can be calculated from their wave functions once their initial states are given. The continuity equation guarantees the integrity of the system information during the evolution of trajectories. In recent years, Bohmian trajectories of photons have been observed with the development of experimental techniques [15–17].

B. Momentum expectation method

Besides the BM approach, we can also obtain the momentum of trajectories by other means. We can transform wave function, \( \psi(r) \), into momentum space,

\[ \varphi(p) = \frac{1}{(2\pi\hbar)^{3/2}} \int d^3r \exp(-i\mathbf{k} \cdot \mathbf{r}) \psi(r). \]

(6)

The momentum space wave function \( \varphi(p) \) is a superposition of momentum eigenstates. So, it is convenient to obtain the expectation value of momentum [18],

\[ \langle p \rangle = \int dp \varphi^*(p) p \varphi(p). \]

(7)

Accordingly, quantum trajectories can be calculated from this momentum expectation. Compared with the BM method, which calculates the velocity of each position of the trajectory, the ME method calculates the mean velocity of each trajectory. Therefore, it is an approximate method which is faster for calculation but less portable than the BM method.

C. EBSD simulation method

We now consider the trajectory simulation method of EBSD. In a crystal, the wave function can be expressed as a superposition of Bloch waves [19],

\[ \psi(r) = \sum_j A^{(j)} \sum_g c_g^{(j)} \exp[i(k^{(j)} + g) \cdot r], \]

(8)

where the expansion coefficients \( A^{(j)}, c_g^{(j)} \), and the wave vectors \( k^{(j)} \) are to be solved. This is a typical problem discussed by Bethe in 1928 [20]. The lattice potential is periodic so that it is expanded as a Fourier series, \( V(r) = \sum_{\mathbf{g}} V_g \exp(i\mathbf{g} \cdot \mathbf{r}) \). By substituting the Fourier series into the Schrödinger equation together with the wave function in Eq. (8), the Bethe dynamic equation is obtained as,

\[ \left[ K^2 - (k^{(j)} + g)^2 \right] c_g^{(j)} + \sum_{\mathbf{h} \neq g} V_{\mathbf{g} - \mathbf{h}} c_h^{(j)} = 0. \]

(9)

Here \( K \) is the wave vector of the incident electrons inside the crystal and \( K^2 = \chi^2 + V_0 \), where \( \chi \) is the wave vector of the incident electrons in vacuum and \( V_0 \) is the mean inner potential of the crystal. That is, when the calculation conditions are determined, \( K, \chi, \) and \( V_0 \) can be calculated directly.

The solution to Eq. (9) is described elsewhere [21–23], so here we only give a synopsis. In the EBSD simulation, the Bloch wave vector \( k^{(j)} \) is decomposed as \( k^{(j)} = K + \lambda^{(j)} \hat{n} \), where \( \hat{n} \) is a unit normal vector of the crystal surface. Then in the case of high-energy electron approximation, Eq.
can be transformed into an eigenvalue equation,
\[ \mathbf{B} \mathbf{C}^{(j)} = \lambda^{(j)} \mathbf{C}^{(j)}, \]
where \( \mathbf{C}^{(j)} \) is a column vector containing \( C_{gg}^{(j)} \), and \( \mathbf{B} \) is a matrix with its diagonal elements,
\[ B_{gg} = -\frac{g^2 + 2 \mathbf{K} \cdot \mathbf{g}}{2}\mathbf{n} \cdot (\mathbf{K} + \mathbf{g}), \]
and off-diagonal elements,
\[ B_{gh} = \frac{V g - h}{2}\mathbf{n} \cdot (\mathbf{K} + \mathbf{g}). \]
When \( \mathbf{B} \) is determined, the eigenvalues \( \lambda^{(j)} \) and the eigenvectors \( \mathbf{C}^{(j)} \) can be calculated. Supposing that \( \mathbf{C} \) is a matrix \( [21] \), whose columns are \( \mathbf{C}^{(j)} \). Then \( \lambda^{(j)} = \mathbf{C}^{-1} \), where \( \mathbf{C}^{-1} \) is the \( j \)-th element in the first column of \( \mathbf{C}^{-1} \).

With all the coefficients computed, the wave function of incident electrons can be obtained from Eq. (8). Then the momentum of electrons can be reckoned by the BM method or the ME method aforementioned, and the trajectories can be derived by the integral,
\[ \mathbf{r}(t) = \mathbf{r}(0) + \int_{0}^{t} \mathbf{v}(t') dt', \]
where \( \mathbf{v} = \mathbf{p}/m \) is the velocity field of electrons.

In the EBSD simulation, only the backscattered electrons are considered. It is a good approximation to treat the backscattered electrons as emitted from a point source inside the crystal and neglect the coherent diffraction from the incident beam \([1, 6]\). In the present trajectory picture, electron trajectories are generated randomly as particles like in a single-electron experiment instead of as a spherical wave function. In this way, we can study both the particle nature and the wave nature of electrons in EBSD. Figure 1 is a schematic of quantum trajectories (cyan arrows) of backscattered electrons inside a crystal (red balls).

III. RESULTS AND DISCUSSION

A. Simulation of single electron experiment

Single electron experiment is a typical kind of experiment to reveal the wave-particle duality of electrons \([24]\). Here we take a molybdenum crystal as an example. Inelastic scattering is considered by calculating the imaginary part of the crystal potential \([25, 26]\) through inelastic mean free path (IMFP) \([27]\). Electron trajectories with the energy of 20 keV are generated one by one randomly at a depth of 20 nm underneath the crystal surface. We calculate the quantum trajectories and count them on a fluorescent screen which is parallel to the (100) crystal plane after they move out of the crystal. The position distributions of the trajectories on the screen are displayed in Figure 2.

Figure 2(a) shows \( 10^2 \) trajectories that are randomly distributed without any feature. This is a probabilistic behavior of a small number of electrons. As the number of electron trajectories increased to \( 10^3, 10^4, \) and \( 10^5 \) [Figure 2(b–d)], features of EBSD pattern appear gradually as a statistical behavior of many electrons. In Figure 2(d), several characteristic bands show up. Then by this simulation, we intuitively reproduce the transformation of the probabilistic behavior to the statistical behavior of pattern formation. From the perspective of the quantum trajectory theory, these behaviors originate from the uncertainty of the initial velocity of electrons.

It is necessary to stress that the concept of quantum trajectory is different from that of classical trajectory. Quantum trajectories indicate an average behavior of an ensemble of electrons, rather than constraining each electron to follow a precise trajectory. In other words, a quantum trajectory represents the most probable path of a series of electrons incident at the same initial position.

B. EBSD pattern

With the increase of the number of trajectories, the characteristic information of the diffraction pattern gradually
appears on the fluorescent screen. Here we have simulated three typical structures, i.e., gold (100) (fcc), molybdenum (100) (bcc), and carbon (100) (diamond) with a depth of 50 unit cells. The energy of the electrons in each material is 20 keV. The fluorescent screen is parallel to the (100) crystal planes. Figure 3 gives the trajectory representation of EBSD pattern of Au, Mo, and C. Each image shows the characteristic Kikuchi bands, but the bands are getting clearer from Figure 3(a) to 3(c) because of inelastic processes. That is, the longer the IMFP is, the clearer the Kikuchi bands are.

Note that the intensity of EBSD pattern cannot be displayed well with only the position distribution of trajectories. Consequently, density distribution is desired. Figure 4 is the EBSD pattern of Mo (100) crystal. Figure 4(a) is the density distribution calculated by the BM method, Figure 4(b) is an experimental pattern [28], and Figure 4(c) is the density distribution calculated by the ME method. Compared with the experimental pattern, both simulation results reproduce the diffraction contrast of EBSD and the structure of the characteristic Kikuchi pattern well.

IV. CONCLUSIONS

In this paper, we present two quantum trajectory approaches to the simulation of EBSD. The conventional simulation methods usually start from the wave nature of electrons, which ignores the particle nature, making the intermediate process of scattering invisible. The trajectory methods can combine the wave nature and particle nature. Thus, they can vividly reproduce the formation process of the diffraction pattern, that is, from the probability distribution of a single electron to the statistical distribution of many electrons. Meanwhile, the trajectory approaches agree with experimental results on the characteristic Kikuchi bands of EBSD. Overall, the trajectory methods can accurately simulate EBSD and give an intuitive physical picture, which helps people better understand the interaction between electrons and solids.

Acknowledgments

We thank to Dr. H. M. Li and the supercomputing center of

![Figure 3: EBSD pattern represented by trajectory position distribution. (a) Au (100) (fcc), (b) Mo (100) (bcc), and (c) C (100) (diamond).](image)

![Figure 4: EBSD pattern with intensity; (a) simulated by the BM method, (b) an experimental result [28], and (c) simulated by the ME method.](image)
USTC for the support of parallel computing. The work was supported by the National Key Research and Development Project (2019YFF0216404) and Education Ministry through “111 Project 2.0” (BP0719016).

Note

This paper was presented at the 12th International Symposium on Atomic Level Characterizations for New Materials and Devices ’19 (ALC ’19), in conjunction with the 22nd International Conference on Secondary Ion Mass Spectrometry (SIMS-22), Miyako Messe, Kyoto, Japan, 20–25 October, 2019.

References

[1] A. J. Schwartz, M. Kumar, B. L. Adams, and D. P. Field (Eds.), *Electron Backscatter Diffraction in Materials Science* (Springer, Boston, 2009).

[2] L. Reimer, *Scanning Electron Microscopy: Physics of Image Formation and Microanalysis* (Springer, Berlin, Heidelberg, 1998).

[3] S. Nishikawa and S. Kikuchi, *Nature* 121, 1019 (1928).

[4] S. Nishikawa and S. Kikuchi, *Nature* 122, 726 (1928).

[5] W. Kossel, *Ann. Phys.* 417, 512 (1936).

[6] A. Winkelmann, C. Trager-Cowan, F. Sweeney, A. P. Day, and P. Parbrook, *Ultramicroscopy* 107, 414 (2007).

[7] J. L. Allen and C. J. Rossouw, *Phys. Rev. B* 39, 8313 (1989).

[8] C. J. Rossouw, P. R. Miller, T. W. Josefsen, and L. J. Allen, *Philos. Mag. A* 70, 985 (1994).

[9] L. De Broglie, *Ann. Phys.* 10, 22 (1925).

[10] D. Bohm, *Phys. Rev.* 85, 166 (1952).

[11] D. Bohm, *Phys. Rev.* 85, 180 (1952).

[12] Z. Ruan, R. G. Zeng, Y. Ming, M. Zhang, B. Da, S. F. Mao, and Z. J. Ding, *Phys. Chem. Chem. Phys.* 17, 17628 (2015).

[13] M. Zhang, Y. Ming, R. G. Zeng, and Z. J. Ding, *J. Microsc.* 260, 200 (2015).

[14] B. Braverman and C. Simon, *Phys. Rev. Lett.* 110, 060406 (2013).

[15] S. Kocsis, B. Braverman, S. Ravets, M. J. Stevens, R. P. Mirin, L. K. Shalm, and A. M. Steinberg, *Science* 332, 1170 (2011).

[16] D. H. Mahler, L. Rozema, K. Fisher, L. Vermeyden, K. J. Resch, H. M. Wiseman, and A. Steinberg, *Sci. Adv.* 2, e1501466 (2016).

[17] H. M. Wiseman, *New J. Phys.* 9, 165 (2007).

[18] L. Cheng, Y. Ming, and Z. J. Ding, *New J. Phys.* 20, 113004 (2018).

[19] R. G. Zeng and Z. J. Ding, *Surf. Sci.* 608, 102 (2013).

[20] H. Bethe, *Ann. Phys.* 392, 55 (1928).

[21] S. S. Sheinin and B. E. Jap, *Phys. Status Solidi B* 91, 407 (1979).

[22] H. S. Kim and S. S. Sheinin, *Phys. Status Solidi B* 109, 807 (1982).

[23] W. Qian, J. C. H. Spence, and J. M. Zuo, *Acta Crystallogr.* A 49, 436 (1993).

[24] A. Tonomura, J. Endo, T. Matsuda, T. Kawasaki, and H. Ezawa, *Am. J. Phys.* 57, 117 (1989).

[25] S. M. Goldberg, R. J. Baird, S. Kono, N. F. T. Hall, and C. S. Fadley, *J. Electron Spectrosc. Relat. Phenomena* 21, 1 (1980).

[26] J. Rundgren, *Phys. Rev. B* 59, 5106 (1999).

[27] H. Shinotsuka, S. Tanuma, C. J. Powell, and D. R. Penn, *Surf. Interface Anal.* 47, 871 (2015).

[28] E. Langer and S. Däbritz, *Phys. Status Solidi C* 4, 1867 (2007).

All articles published on e-J. Surf. Sci. Nanotechnol. are licensed under the Creative Commons Attribution 4.0 International (CC BY 4.0). You are free to copy and redistribute articles in any medium or format and also free to remix, transform, and build upon articles for any purpose (including a commercial use) as long as you give appropriate credit to the original source and provide a link to the Creative Commons (CC) license. If you modify the material, you must indicate changes in a proper way.