Summit to: Computational material sciences and Monte Carlo methods

Study of Atomic Resolution of Secondary Electron Imaging in STEM Using a Quantum Trajectory Monte Carlo Method

Z. Ruan[1], Z.J. Ding[1*]

[1]Hefei National Laboratory for Physical Sciences at Microscale and Department of Physics, University of Science and Technology of China, Hefei, Anhui 230026, P. R. China

EXTENDED ABSTRACT: The quantum trajectory Monte Carlo simulation method is developed to describe the interaction between electron beam and crystal in electron microscopy and spectroscopy. Compared with the classical Monte Carlo simulation, this novel method combines the Bohmian quantum trajectory method [1], which treats electron elastic scattering and diffraction in a crystal, with a Monte Carlo sampling of electron inelastic scattering behaviors along quantum trajectory paths. The electron scattering and secondary electron generation process in crystals by a focused incident electron beam has been studied in detail with this method, which reveals the imaging mechanism of the atomic resolution secondary electron image recently experimentally achieved with a scanning transmission electron microscope. In this method, at first the Bohmian quantum trajectories have been calculated through a wave function which is derived from a numerical solution of the time-dependent Schrodinger equation with a multislice method. Based on the impact parameter dependent inner-shell excitation cross section, the Monte Carlo sampling of ionization events produced by incident electron trajectories travelling along atom columns was achieved for excitation of high energy knock-on secondary electrons. Following cascade production, transportation and emission processes of true secondary electrons at very low energies is traced by a classical Monte Carlo simulation method to generate simulated image signals. The highly consistence of the simulated image for a Si (110) crystal with the experimental image sucessfully reveals that the inner-shell ionization events generated by a high energy electron beam is dominant mechanism for atomic resolution of secondary electron image.

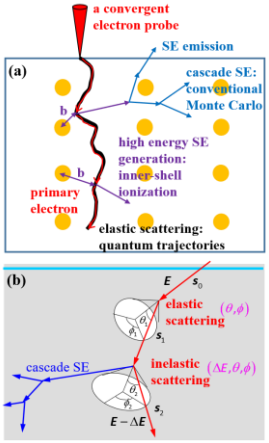

Fig. 1 The illustration of quantum trajectory Monte Carlo method.

Keywords: secondary electron image; electron-crystal interaction; Monte Carlo

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BIOGRAPHY

* Corresponding author: zjding@ustc.edu.cn.

Zhu Ruan has obtained Ph.D in Physics from University of Science and Technology of China, in 2015 (with Prof. Zejun Ding) and performed postdoctoral studies at Institute of Chemistry, Hebrew University of Jerusalem, Israel during 2016-2018 (with Prof. Roi Baer). She is now a senior algorithm engineer in physics of semiconductor device at Nine Cube, a start-up EDA company in China.