Recent development of Monte Carlo method for electron spectroscopy and electron microscopy

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Monte Carlo simulation method has been widely used to material analysis by means of electron probe microanalysis, surface electron spectroscopy and electron microscopy. We have recently developed a reverse Monte Carlo (RMC) method to derive optical constants of solids from reflection electron energy loss spectroscopy spectra with the use of fast parallel computation. The method combines the Monte Carlo simulation of surface excitation in REELS spectrum with a Markov chain Monte Carlo sampling of oscillator strength parameters. In addition, to take account of electron diffraction effect in a crystalline sample we have developed a novel type of electron trajectory simulation technique, i.e. the quantum Monte Carlo (QMC) method. The principle of the method is to combine the Bohmian quantum trajectory calculation of electron elastic scattering with conventional Monte Carlo sampling of electron inelastic scattering along trajectory path. The QMC method holds the accuracy of quantum mechanics while still keeping the classical particle trajectory picture for convenience to practical application. As an example, the atomic resolution SEM imaging mechanism has been exploded with the method. The QMC method is expected to play important role to future electron microscopic and spectroscopic analysis of nanostructures.

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