**Extracting Optical Properties from Reflection Electron Energy-Loss Spectroscopy Spectra by Reverse Monte Carlo Method**

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Optical properties of solids are of interest both in fundamental research and applied fields. Although an existing database of optical constants compiled by Palik has been widely used, there still lack sufficient data in intermediate photon energies for some materials, which is mostly due to the drawbacks of using a light probe in traditional optical methods like reflectance and absorption spectroscopy. Recently research focus has been put on the derivation of optical constants with reflection electron energy loss spectroscopy (REELS). For this we have developed a new analytical tool, the reverse Monte Carlo method (RMC), to obtain optical constants from the measured reflection electron energy-loss spectrum [1]. The method combines the Monte Carlo simulation of REELS spectrum with a Markov chain Monte Carlo calculation of oscillator parameters describing the dielectric function ε(ω,q) of a solid. In the Monte Carlo simulation of REELS spectrum a depth-dependent differential inverse inelastic mean free path model is adopted for energy loss distribution of the electrons; elastic scattering and multiple scattering effects are also included. The principle of RMC method is to utilize an iterative process to seek the optimal oscillator parameters, which are used to calculate differential inverse inelastic mean free path, by comparing the Monte Carlo simulated REELS spectrum with the measured one. The energy loss function, Im{-1/ε(ω,q)}, is used as an input for modeling electron inelastic scattering through both bulk excitation and surface excitation. In each iteration step, the oscillator parameters are then updated taking into account of the least-square residuals between the simulated and the measured REELS spectra, employing a Markov chain Monte Carlo sampling procedure.

We have studied optical properties of several transition metals and lanthanides including Fe, Ni, Pd, Co, Cr, Ir, Sm and Tb in a wide energy loss (or photon energy) range of 0-100 eV. The REELS experimental spectra were recorded by a homemade electron spectrometer at ATOMKI & MFA. Optical data are then obtained by the RMC method. The oscillator strength-sum rule and perfect-screening-sum rule have been applied to examine the reliability of the data. A comparison of our results with the data from literatures has also been made.

**References:**

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