Determination of Optical Properties of Tungsten from Reflection Electron Energy Loss Spectroscopy Spectra by Reverse Monte Carlo Method

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Tungsten is an ideal choice for electron gun filaments in scanning electron microscopy (SEM) and tips for scanning tunneling microscopy (STM) as it possesses the highest melting point and tensile strength among all pure metals. Employing the reverse Monte Carlo (RMC) method, which is the combined technique of Monte Carlo (MC) simulation of reflection electron energy loss spectroscopy (REELS) spectrum and the Markov chain Monte Carlo (MCMC) updating of oscillator parameters, we have precisely determined the energy loss function (ELF) of tungsten in the energy loss range of 0.1-110 eV at the incident electron energies of 1 keV, 2 keV and 3 keV from experimental REELS spectra. The final obtained simulation result of the three investigated energies demonstrate excellent agreement with the experimental spectrum in Fig. 1(a). Furthermore, we have successfully differentiated between bulk and surface contributions to the REELS spectra in Fig. 1(a). The simulated bulk REELS spectra reveal peaks at ~25.5 eV, 43 eV and 53 eV, which were recognized as bulk plasmon excitations. And features located at ~ 2 eV, 10 eV and 21 eV were identified as surface plasmon excitations. We have obtained a high accurate averaged optical ELF over the three energies whose relative errors of the perfect-screening sum rule and oscillator-strength sum rule were ~0.70% and 0.68%, respectively. Fig. 1(b) presents the averaged optical ELF and the comparison with the literature data [1,2,3]. Applying Kramers-Kronig relation, we have calculated the optical constants and dielectric function of tungsten from the averaged optical ELF derived by the RMC method, as illustrated in Figs. 1(c) and 1(d). The high accuracy of the derived ELF, optical constants and dielectric function will be beneficial for their practical applications in material science.

Keywords： tungsten; reflection electron energy loss spectroscopy; reverse Monte Carlo; energy loss function

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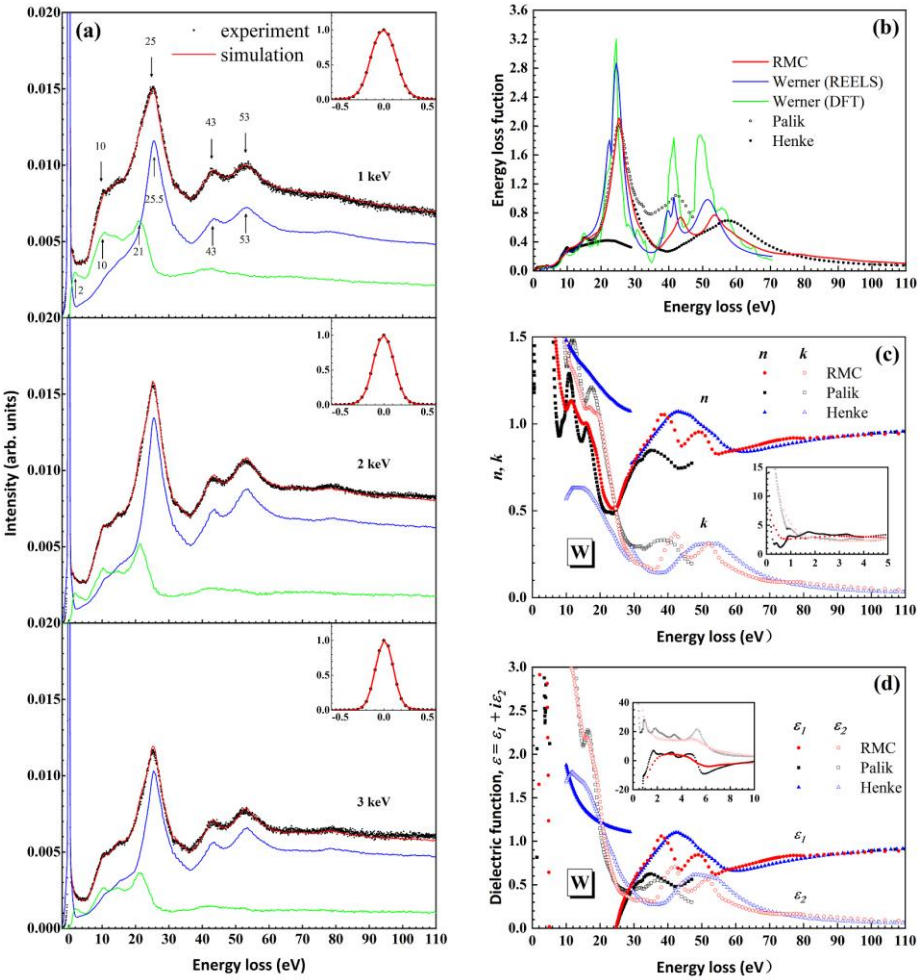

Figure 1. (a) The simulated REELS spectra (red lines) and measured spectra (black lines) of tungsten at 1 keV, 2 keV and 3 keV. Contributions from surface and bulk excitations are separated from the simulated total spectrum and shown by the green and blue lines, respectively. The inset shows the elastic peak for convolution of the simulated spectrum. (b) Comparison of the averaged ELF obtained from the RMC method (red line) with Werner's REELS data (blue line) [1], Werner's DFT data (green line) [1], Palik's compiled data (open circles) [2], and Henke's data (solid circles) [3]. (c) Plots of the refractive index n (red solid circles) and extinction coefficient k (red open circles) derived from the RMC method in comparison with Palik's data (black squares) and Henke's data (blue triangles). (d) Plots of the real part ε_1 (red solid circles) and imaginary part ε_2 (red open circles) derived from the RMC method in comparison with Palik's data (black squares) and Henke's data (blue triangles).

BIOGRAPHY

Zhen Li has completed her undergraduate from Applied Physics Department, School of Science, Dalian Maritime University, China in 2021. She is now the PhD student of Physics Department, School of Physics, University of Science and Technology of China.