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Revision of optical property of silicon by a reverse Monte Carlo analysis of reflection electron energy loss spectroscopy spectra

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Synopsis The energy loss function (ELF) of silicon in a wide photon energy region (0-200 eV) was derived from reflection electron energy loss spectroscopy spectra with a theoretical analysis of the measured data. The accuracy of our result was justified by using the f- and ps-sum rules. Based on the new ELF, individual contributions of surface excitation and the bulk excitation to the REELS spectrum have been separated, and multi-scattering effect in the reflection electron energy loss spectroscopy spectrum has been studied in detail.

In recent years a well-established technique based on the reflection electron energy loss spectroscopy (REELS) has been developed to obtain optical constants in a wide range of electron energy loss. The REELS method does not require a complicated process for preparation of samples and the incident electron energy is usually around a few keV. However, the REELS spectrum usually contains not only bulk excitation but also surface excitation. To remove the surface excitation effect and multiple scattering effect from the REELS spectrum in data analysis, Da et al. [1] developed a reverse Monte Carlo (RMC) method for the derivation of the energy loss function (ELF) and thereby the dielectric function and optical constants of solids in a much wider photon energy range than that of the usual optical measurements [2,3]. The RMC method combines a Monte Carlo modelling of electron transportation for REELS spectrum simulation with a Markov chain Monte Carlo calculation of parameterized ELF. During the Monte Carlo simulations we used the Mott cross section with Thomas–Fermi–Dirac atomic potential to describe the electron elastic scattering, and the dielectric function theory for the description of the electron inelastic scattering processes [2]. The REELS spectra of Si were measured with primary electron energies at 3000, 4000 and 5000 eV in an energy-loss range of 0-200 eV. Then the RMC technique was applied to extract the ELF of Si. The reliability of the obtained data has been confirmed by applying the Thomas-Ritchie-Kuhn and the perfect-screening sum rules. Figure 1 shows that the agreement between the final simulated REELS spectra (blue line) and experimental REELS spectra (red dots) on the absolute intensity scale is excellent, covering the energy loss range from the elastic peak down to an energy loss of 100 eV, for the primary energy of 4000 eV. The inset of the figure shows the ELF obtained by the RMC method (blue line) in comparison with the results in databases of Palik (red circles) and Henke (black squares), which provides the revision of optical constants derived from optical measurements particularly around 10 eV.

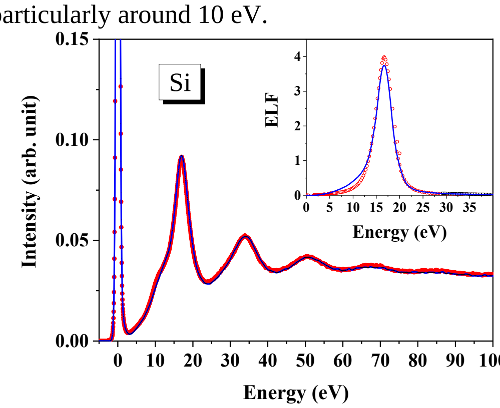

Figure 1. The REELS spectra and ELF of Si.

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