Optical Properties of Sm and Tb Derived from REELS Spectra

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In this study we employed the recently developed reverse Monte Carlo (RMC) method [1, 2] to extract the energy loss function (ELF) and the optical constants (i.e. refractive index and extinction coefficient) and dielectric function, for lanthanide elements, Sm and Tb. The RMC method, combining with the measured reflection electron energy loss spectroscopy (REELS) spectra, has proved advantageous in its simplicity of the measurement on experimental operation and for minimal sample preparation requirements. Various REELS spectra were measured under different experimental conditions, and the RMC method was applied for calculations to obtain a wide range of optical properties. The final outcomes of ELFs for Sm and Tb in the loss energy range up to 180 eV.

To align the simulated spectrum with the experimental one, the elastic peak (i.e. the zero-loss peak) is adjusted through convolving a set of Gaussian functions. Both spectra are normalized to the elastic peak, as depicted in Fig. 1. [3-7] Surface and bulk contributions can be distinguished in Fig. 1(a). The illustration in Fig. 1(b) shows the data taken by Miller et al. and Krizek et al. [5, 6] at room temperature from the Palik database [7]. In the infrared region, the ELF of the Tb is relatively small, and all available data is very close. In the intermediate energy loss region there is a relatively limited amount of available data regarding the ELF, for instance, results obtained by Colliex et al. [3] by using transmitted energy loss spectra only encompass data below 45 eV, making it difficult to seamlessly integrate with the results by Henke et al. [4]

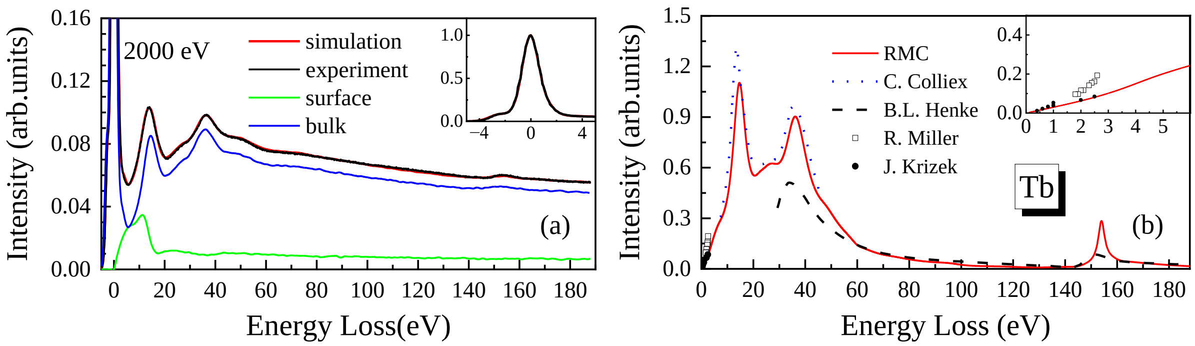

Figure 1. (a) Comparison of the REELS spectra obtained through RMC with experiment at 2000 eV. (b) Comparison of ELFs obtained in this work with literature data.

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In this study, the deficiency is addressed by incorporating ELF data obtained through RMC. Comparisons with other results demonstrated favorable consistency, emphasizing the reliability of the RMC method in accurately characterizing the optical properties of materials. Notably, the trends of ELF and optical constants for Sm and Tb appeared similar, suggesting their common characteristics for electronic excitation. ELF and optical constants for Sm will be explained in detail in the report.

The complex dielectric function and the optical constants were also obtained for the first time as complete curves covering from the infrared region to the soft x-ray photon energy region based on the Kramers-Kronig relations [8]. The optical constants obtained in this work have a consistent trend compared with those in the Henke database. The accuracy of the obtained ELF and optical constants was rigorously validated through the application of the *ps*- and *f*-sum rules [9], showing relative errors are within a narrow range smaller than one percent. The presented methodology addresses limitations of traditional optical measurement techniques, providing a robust and efficient approach for exploring the optical behavior of lanthanides.

Keywords： optical constants; samarium; terbium; reverse Monte Carlo; reflection electron energy loss spectroscopy

REFERENCES

[1] B. Da, S. F. Mao, Y. Sun and Z. J. Ding, *J. Surf. Sci. Nanotechnol.* **10** (2012) 441.
[2] B. Da, Y. Sun, S. F. Mao, Z. M. Zhang, H. Jin, H. Yoshikawa and S. Tanuma, *J. Appl. Phys.* **113** (2013) 214303.
[3] C. Colliex, M. Gasgnier and P. Trebbia, *J. Phys*. **37** (1976) 397.
[4] B. L. Henke, E. M. Gullikson and J. C. Davis, *At. Data Nucl. Data Tables* **54** (1993) 181.
[5] R. Miller, L. Julien and A. Taylor, *J. Phys. F: Met. Phys*. **4** (1974) 2338.
[6] J. Krizek and K. Taylor, *J. Phys. F: Met. Phys*. **5** (1975) 774.
[7] E.D. Palik, Handbook of Optical Constants of Solids, Academic Press. Vol. 3, (1998).
[8] H. Xu, B. Da, J. Tóth, K. Tőkési, and Z.J. Ding, *Phys. Rev. B* **95**(2017) 195417.
[9] S. Tanuma, C.J. Powell, D.R. Penn, *J. Electron Spectrosc. Relat. Phenom.* **62** (1993) 95-109.

BIOGRAPHY

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