Summit to: Materials Database Construction

Improved Reverse Monte Carlo Analysis of Optical Property of Fe and Ni from Reflection Electron Energy Loss Spectroscopy Spectra

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EXTENDED ABSTRACT: The energy loss functions (ELFs) of Fe and Ni have been derived from measured reflection electron energy loss spectroscopy (REELS) spectra by the reverse Monte Carlo analysis [H. Xu et al., *Phys. Rev. B*, **95**, (2017) 195419; H. Xu et al., *Nucl. Instr. Meth. B*. **406**, (2017) 475-481]. In this work, we make some improvements for the two metals respectively. For Fe, we update our previous ELFs at primary electron energy of 2000 eV and 3000 eV in a wider photon energy region (0-180 eV) with a better accuracy, which is verified by sum rules. About Ni, we supplement the ELF at primary energy of 5000 eV besides improving the accuracy of 3000 eV. Moreover, we employ the more accurate ELFs to analyze the optical constants and dielectric functions of the two metals compared with other references.

Keywords： reverse Monte Carlo; reflection electron energy loss spectroscopy; optical property

REFERENCES

[1] H. Xu, B. Da, J. Tóth, K. Tőkési and Z. J. Ding, *Phys. Rev. B*, **95**, (2017) 195417

[2] H. Xu, L. H. Yang, J. Tóth, K. Tőkési, B. Da and Z. J. Ding, *Nucl. Instr. Meth. B*, **406**, (2017) 475-481

[3] L. H. Yang, K. Tőkési, J. Tóth, B. Da, H. M. Li and Z. J. Ding, *Phys. Rev. B*, **100**, (2019) 245209

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