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Multiple-scattering approach to inelastic x-ray scattering calculations¹ J.A. SOININEN, U. of Helsinki, A.L. ANKUDINOV, J.J. REHR, U. of Washington — We present an implementation of the real-space multiple-scattering (RSMS) approach for calculations of non-resonant inelastic x-ray scattering (NRIXS) from core-electrons, which is also termed x-ray Raman scattering (XRS). The RSMS approach has been used extensively to model x-ray absorption spectra from deep core levels, including both the fine structure and near-edge behavior. This *ab initio* method includes final state self-energy and lifetime effects as well as an approximate treatment of the core-hole interaction. Moreover, the method is applicable to aperiodic or periodic systems alike. The momentum transfer dependence of the XRS is related to the dynamic structure factor $S(\vec{q}, \omega)$. The results for XRS at different momentum transfers yield information concerning local symmetries of the excited states through changes in the spectral weight of mono-pole, dipole, quadrupole, and higher couplings. Our results are compared both with experiment and with other theoretical calculations. Our near edge calculations are in agreement with previous calculations, and we show how the approach can also be used to calculate the fine structure.

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