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Relativistic real-space multiple scattering calculations of EELS[1]
K. JORISSEN, U. Antwerp, J.J. REHR, A. SORINI, U. of Washington, Z.H. LEVINE, NIST — We present an extension of the real space multiple scattering code FEFF8 for *ab initio*, relativistic calculations of electron energy loss spectra (EELS), which is applicable both to periodic and non-periodic systems. The approach explains the observed relativistic shifts in the magic angle. [2] In addition, the method can account for experimental parameters such as collection and convergence angles of the microscope and sample orientation. We also discuss relativistic effects on inelastic electron scattering including the density correction to the stopping power. Our results are compared with other approaches and with experiment.

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[2]B. Jouffrey, P. Schattschneider and C. Hebert, Ultramicroscopy **102**, 61 (2004).

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