Abstract Submitted
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Theoretical description of the white lines in 3d transition metals
KOFI NUROH, Kent State University — The $3d \rightarrow 2p_j$ $(j = 3/2,\ 1/2)$emission lines in the 3d transition metals ^{21}Sc through ^{27}Ni have been studied using a theoretical model based on autoionization and characteristic decay events following electron impact ionization of a core electron in solids. The theory primarily hinges on the Bethe-Born formalism of inelastic scattering of electrons on atoms with the inclusion of correlation effects via many-body perturbation techniques. The $2p^5 3d^{n+1}$ intermediate resonant configuration is diagonalized to provide the multiplet splitting and their corresponding intensities. By analyzing the relative magnitudes of the electrostatic and magnetic interactions of the $2p$and $3d$electrons, it is found that LK coupling is suitable for the systems Sc, Ti, and V, while jK coupling is appropriate for Cr to Ni. Applying the dipole approximation to the Coulomb transition matrix elements, the calculated electron-energy-loss- spectra separate into two distinct manifolds that arise from the $2p_{3/2}$ and $2p_{1/2}$ levels, namely, the white lines, and the calculations compare very well with measurements for x-ray absorption spectra.
Reference: K. Nuroh, Physical Review B 78, 245116 (2008).

Kofi Nuroh
Kent State University

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