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MODEL SIMULATIONS OF THE SUB-BANDGAP ENERGY LOSS SATELLITES IN SI 2P AND BE 1S RIXS SPECTRA IN BERYLLIUM COMPOSITE COMPOUNDS

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Resonant X-Ray inelastic scattering spectra have been measured in BeO [1], phenakite and chrysoberyl crystals with the excitation energy near the beryllium K edge.

The experimental RIXS spectra excited in the vicinity of the core resonance show two principal features: the scattering on a valence exciton (this band verges into the characteristic Kα emission at higher excitation energies), and a remarkably strong energy loss side-band (more than 6 eV wide) to the elastic scattering peak. This side-band arises from the so-called participator emission where the core photoexcited electron makes a radiative transition back to the core hole losing some energy in the process. This phenomena is similar to the Raman shift seen in optical spectroscopy, but in the soft x-ray regime the core hole lifetime is short and the width is comparable to the vibrational quantum so one expects interference effects too.

To gain further insight to this process, electronic transitions in a system with a single symmetric vibrational mode have been modeled. To separate the electronic and the nuclear motion the Born-Oppenheimer approximation together with Franck-Condon principle for transitions has been used. The shape of the potential energy curves has been described by Morse potentials.

The calculated emission spectra are based on the Kramers-Heisenberg formula.

$$\sigma(h\nu, f) \propto \left| \sum_i \frac{\langle f_n i_n \rangle \langle i_n g_n \rangle}{h\nu - (E_i - E_g) - \frac{i\Gamma}{2}} \right|^2$$

The phonon relaxation has been simulated empirically by „smearing“ the photoabsortion-populated vibrational levels with lower levels using an exponential distribution.

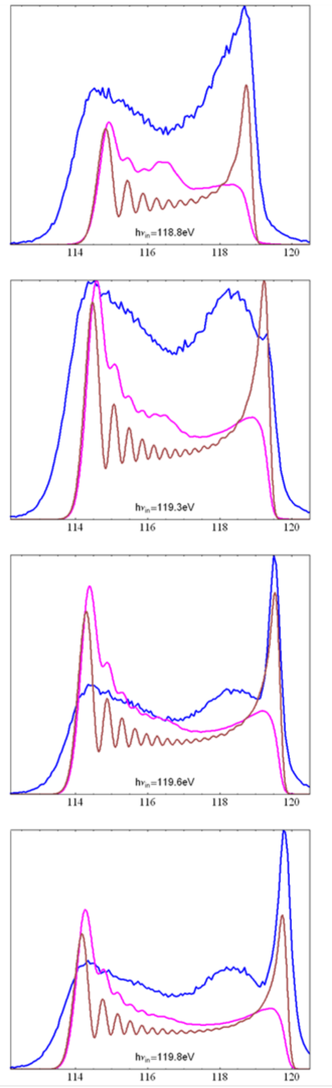

Figure 1. X-Ray emission spectra of BeO. Blue lines show the experimental participator emission spectra, brown lines show the modeled spectra and purple line is the empirical two-step model which simulates phonon relaxation.

References

1. Käämbre, T., et al. "Resonant Inelastic X-Ray Scattering at the Be 1s Edge in BeO." *J. Electron Spectrosc. Relat. Phenom.* 156-158 (2007): 299-302.