Study of the Dynamic and Static Electronic and Magnetic Structures in $NiS_{2-x}Se_x$ Using Inelastic and Elastic X-ray Scattering

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Resonant inelastic x-ray scattering (RIXS) is a powerful probe of the low-energy excitations in a solid which measures the energy loss and momentum transfer of scattered x-rays. We have measured the q dependent RIXS spectra of a single crystal of NiS_2 along the [111] direction. The measurements were performed at the Taiwan beamline BL12XU at SPring-8. In the RIXS experiment the incident beam was monochromatized using the Si (111) DCM and two Si (400) channel cuts; the spectra were measured using a 2-m radius spherically bent Si (551) analyzer. The total energy resolution was about 0.3eV.

The RIXS spectra obtained for the NiS_2 single crystal are displayed in Figure 1 with various excitation energies across the Ni K-edge. Here the transferred energy is defined as $\Delta E=E_1-E_2$; in which E_1 is incident excitation photon energy and E_2 is emitted photon energy. The center of the elastic peak is set to zero. The broad and rather strong peak in the high transferred energy side is observed to shift towards higher energy proportional to the incoming of the incident energy. This feature is attributed to the excitation of a Ni *3d* electron into the Ni 4*p* states, and can be also referred to the $K\beta_{2,5}$ valence band emission. The $\Delta E \cong 5$ eV peak can be assigned to a charge-transfer excitation between the S and Ni sites. The maximum of the resonant enhancement of this feature is reached when the incident energy is set to 8344 eV.

Figure 2 shows the RIXS spectra measured at an incident energy of 8344 eV for different values of the momentum transfer *q* across the first (L[0.5, 0.5, 0.5)]) and second (L'[1.5, 1.5, 1.5]) Brillouin zones along the d^*_{111} direction. From *q*=1.198 $Å^{-1}$ [5/8,5/8,5/8]to *q*=2.1568 $Å^{-1}$[9/8,9/8.9/8 the charge transfer peak energy shifts from ~5 eV to ~5.5 eV while the intensity substantially increases. When *q* is further increased to 4.2 $Å^{-1}$ [2.19,2.19,2.19]both the peak energy and intensity return gradually to values very close with [0.5,0.5,0.5]. This suggests a dispersive behavior of the charge-transfer feature with a period equal to one Brillouin zone. Moreover we also observed that at q=2.1568 $Å^{-1}$ a weak peak at $\Delta E = \sim 10$eV, according to the Platzman et al.'s suggestion that it could correspond to the charge transition from a S $pp\pi^*$ to an unoccupied S $pp\sigma^*$ anti-bonding state.