Table I: Screening electron number in the d-symmetric states inside the muffin-tin sphere at the 3s core-hole site. The radii of the muffin-tin spheres are 2.0 Bohr.

	3s hole spin	$\Delta n_{d\uparrow}$	$\Delta n_{d\downarrow}$	$\Delta n_{d\uparrow} + \Delta n_{d\downarrow}$
Fe	up	-1.44	2.38	0.94
	dn	0.47	0.48	0.95
Co	up	-0.52	1.55	1.03
	dn	0.24	0.75	0.99
Ni	up	0.07	0.87	0.94
	dn	0.26	0.65	0.91

The Fe metal takes a bcc structure. Figures 2 and 3 show DOS's projected onto the states with d symmetry (d-DOS) at the core-hole site for Ni and Co, respectively. The corresponding DOS's for Fe are shown in Fig. 3 in Ref. 19. In these calculations, six k-points are picked up in the irreducible Brillouin zone for super-cell systems. The DOS's calculated with no core-hole are essentially the same as those reported by Moruzzi, Janak and Williams.[25] Table I lists the screening electron number $\Delta n_{d\sigma}$ in the d-symmetric states with spin σ, that is, the difference of the occupied electron number between in the presence and in the absence of the core hole inside the muffin-tin sphere.

On the basis of these one-electron states, we calculate the 3s XPS spectra, by following the procedure describe in Sec. II. Figures 4, 5 and 6 are the spectra thus calculated as a function of the binding energy $\omega_q - \epsilon$ for Ni, Co, and Fe, respectively, in comparison with the experiments.[10,11,13] The spectral shape in Fig. 6 for Fe is slightly different from our previous result (Fig. 4 in Ref. 19), since the present calculation takes full account of excitations up to three e-h pairs in comparison with only up to two e-h pairs in Ref. 19. The spectra are strikingly different between the up-spin channel and the down-spin channel and strongly depend on elements, in good agreement with the experiments. In the following, we explain the origin of these behaviors in relation to one-electron states screening the core hole.

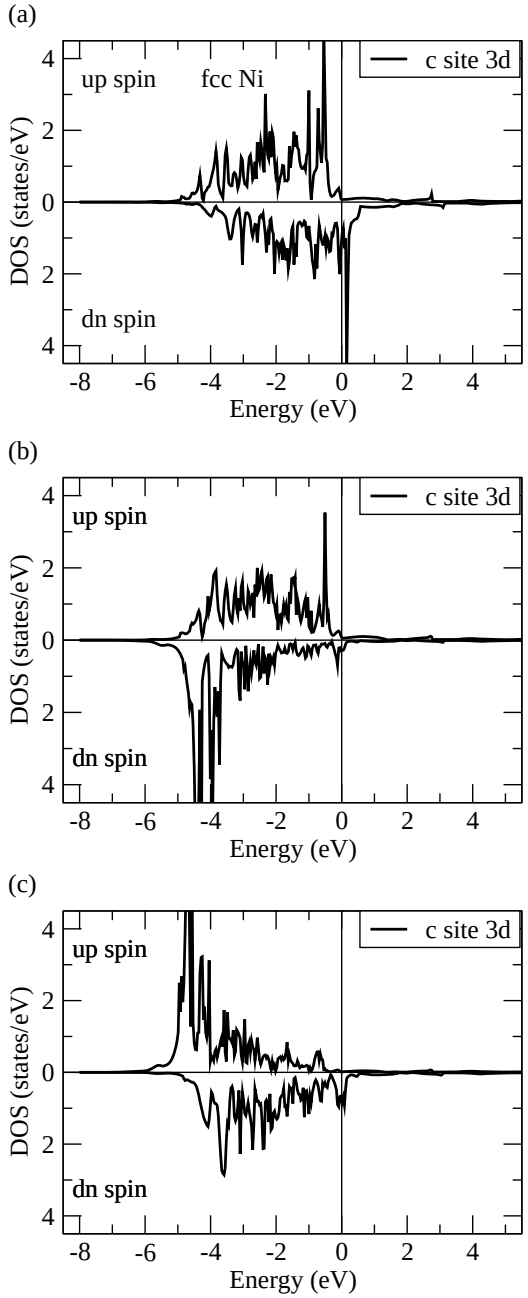

Figure 2: Calculated d-DOS at the core-hole site in the super-cell system in ferromagnetic nickel; (a) d-DOS with no core-hole, (b) d-DOS when the 3s up-spin electron is removed, (c) d-DOS when the 3s down-spin electron is removed.