X-ray Absorption Near-Edge Structure Spectroscopy Research on Electronic Structures and Magnetic Properties of $(Fe_{1-x}Ni_x)_2P$

Chen-Yan Ma (馬陳燕)[1], Ming-Qi Cui (崔明啟)[1], Ling-Yun Jang (張凌雲)[2], Ke-Jin Zhou (周克瑾)[1], Xiang Wu (巫翔)[1], and Wu Ziyu (吳自玉)[1]

[1] Institute of High Energy Physics, The Chinese Academy of Sciences, Beijing, China
[2] National Synchrotron Radiation Research Center, Hsinchu, Taiwan

The M_2P-type structure system with space group $P\bar{6}2m$ are very important in industry for their magnetic characterization, such as Fe_2P, Ni_2P. In the primitive cell, there are two crystallographic positions M(3f), M(3g) and P(2c), P(1b) sites in metal atoms and P atoms respectively. The electronic structures and magnetic properties of Fe_2P, Ni_2P and their compounds $(Fe_{1-x}Ni_x)_2P$ (x=0.1,0.25,0.5) are studied by X-ray absorption near-edge structure (XANES) spectroscopy. The Fe, Ni k-edges XANES spectra were measured at BSRF BL-1W1 and P k-edge was collected at NSRRC BL-16A1 beamlines.

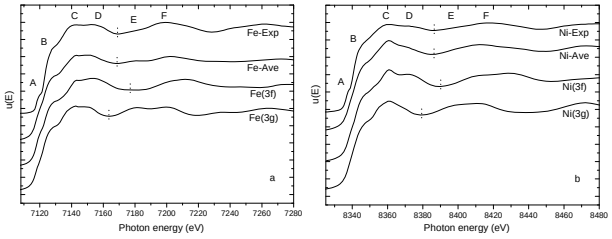

Figure 1. Calculated and experimental k-edge XANES spectra (a)Fe_2P,(b)Ni_2P.

The k-edge XANES spectra of 3g sites and 3f sites in metal atoms were calculated by full multiple-scattering approach (FMS) and the calculated results are in agreement with experiment data. The curves shows that the two sites contribute differently to XANES spectra and D and E points are mostly come from 3f and 3g sites of metal atoms respectively.

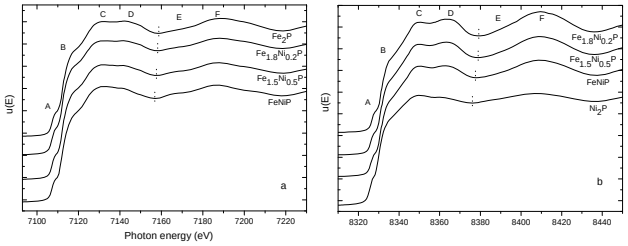

Figure 2. Fe,Ni-K XANES spectroscopy of $(Fe_{1-x}Ni_x)_2P$ (x=0,0.1,0.25,0.5,1) (a)Fe k-edge,(b)Ni k-edge

When Ni atoms are added in Fe_2P, the intensity of D point reduced and E point increased. Combined the calculated conclusion that D and E points are come from 3f and 3g sites, Ni atoms prefers to substitute Fe (3f) sites when introducing Ni atoms.(Fig 2)

In Fig 3, the FWHM of white peak become narrow in P k-edge XANES from Fe_2P(3.8eV) to Ni_2P(2eV), relatived to point B, the intensity of point C increased and the energy position gradually move to high energy. The First-principle Density of States calculations were performed and results show that unoccupied P p-projected DOS of

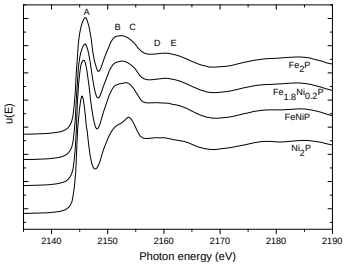

Figure 3. P k-edge XANES of $(Fe_{1-x}Ni_x)_2P$(x=0,0.1,0.5,1)

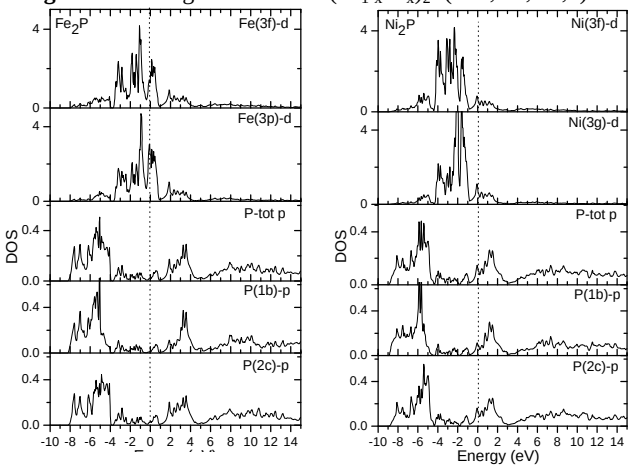

Figure 4. Calculated DOS of paramagnetic Fe_2P and Ni_2P

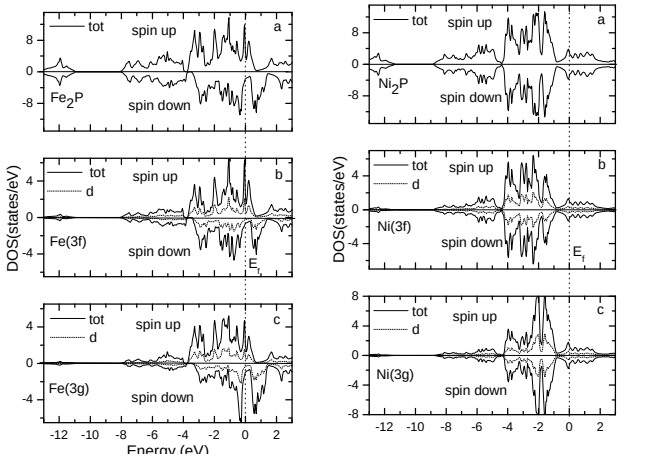

Figure 5. Calculated DOS of ferromagnetic Fe_2P and Ni_2P

paramagnetic Fe_2P and Ni_2P are matched with their K-edge XANES spectra (Fig 4). Compared with DOS of ferromagnetic Fe_2P(Fig 5), it indicates that the magnetism of Fe_2P is mostly affected by Fe(3g) sites. Moreover, the magnetic moments calculated for sites of ferromagnetic Ni_2P approach Zero, which is in coincidence with the conclusion that Ni_2P generally appears paramagnetism.