Electronic and Atomic Structures of Surfaces and Interfaces in Semiconductor Hetero-systems

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Hetero-interfaces play important roles in semiconductor devices. However, they have many problems to be solved, e.g., difficult hetero-epitaxial growth, unstable metallic contact formation, etc. Synchrotron radiation(SR) has such characteristics as high brilliance, variable wavelength, etc. Therefore, it is very useful light source to investigate surfaces and interfaces including thin films. The information on the electronic state of a transition metal silicide film grown on a Si substrate will help us to have a reliable very thin silicide contact formation on a substrate, e.g., Si(100). In order to clarify the origin of this kind of problem, we have been trying to have fundamental knowledge on the formation process and the electronic structure of a transition metal silicide.

PdSi, NiSi and PtSi are transition metal monosilicides with the MnP-type crystal structure. In the monosilicides, the metal(M) atoms (Pd, Ni and Pt) have the same number of valence electrons, i.e., ten electrons. Therefore, we can deduce important information on the relation between the electronic structure and the atomic configurations of these silicides. The soft X-ray emission spectroscopy(SXES) has been used for the study of structural and/or electronic properties of the silicides. Si K_β emission band spectra for the silicides are shown in Fig.1, where the spectrum is considered to reflect Si p electronic state of the valence band density of states(VB-DOS) of the silicides because of the dipole selection rule. Each spectrum is constructed by two peaks which are concluded to be due to the formation of bonding and antibonding states of Si p electrons with metal d electrons[1]. A detailed analysis has shown that the distance between Si and metal atom, i.e., d[Si-M], has an important effect on the peak separation of the two peaks in the Si K_β spectra[1]. Similar intimate relation is found between the spectral shape of the Si $L_{2,3}$ emission and the atomic distance in the silicides[1], where the Si $L_{2,3}$ emission spectrum reflects the Si s or d electronic structure of the VB-DOS. This result indicates that the band structure modification can be performed by manipulating atomic distances in silicides.

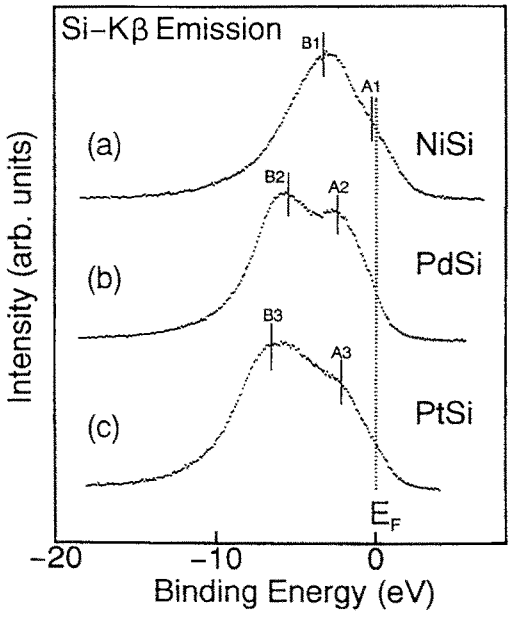

Fig.1 Si K_β emission band spectra for PdSi, NiSi and PtSi[1]

Reference

[1] S.Yamauchi, S.Kawamoto, M.Hirai, M.Kusaka, M.Iwami, H.Nakamura, H.Ohshima and T.Hattori, Phys. Rev. B50, 11564 (1994).