Materials Science-Poland, 37(1), 2019, pp. 116-121
http://www.materialsscience.pwr.wroc.pl/
DOI: 10.2478/msp-2019-0001

X-ray photoelectron spectroscopy (XPS) study of Heusler alloy (Co_2FeAl) interfaced with semiconductor (n-Si) structure

ARVIND KUMAR[1,2,*], P.C. SRIVASTAVA[2]

[1]Department of Physics, Atma Ram Sanatan Dharma College, University of Delhi, Dhaula Kuan, New Delhi-110021, India
[2]Department of Physics, Banaras Hindu University, Varanasi-221005, India

Layered magnetic heterostructures are very promising candidates in spintronics in which the influences of interfaces, surfaces and defects play a crucial role. X-ray photoelectron spectroscopy (XPS) study has been performed for studying in detail the chemical state and electronic structure of Co_2FeAl (CFA) Heusler alloy interfaced with Si substrates. XPS survey scan spectra have clearly shown the presence of Fe, Co and Al signal along with the signal due to Si. The presence of Co, Fe and Al signal confirms the formation of CFA alloy phase. Our XPS results support our previous study [1] on CFA/Si structure in determining the magnetic and transport properties across the interface.

Keywords: *Co_2FeAl; Heusler alloy; XPS; XRD, silicides*

1. Introduction

Heulser alloys, a class of half metallic ferromagnets (HMFs), are potential candidates for spintronic devices having high Curie temperature, large spin polarization and compatibility with compound semiconductors (SCs) [2]. Among the Heusler alloys, Co-based full-Heusler alloys have gained much interest and due to their high Curie temperature higher than room temperature, good lattice matching with major substrates and large magnetic moments, are the most promising candidates to achieve the room temperature (RT) half metallicity [3, 4]. Such promising properties of Co-based, i.e. Co_2YZ type Heusler alloy [5] make it suitable for the use as a ferromagnetic layer in ferromagnetic/semiconductor interfaces for efficient spin injection from the metal side to semiconductor [6]. Having such exceptional properties, Heusler alloys are useful materials for realization of devices based on magnetoresistance (MR) effect. Ferromagnetic/semiconductor interfaces are also promising structures for realizing spintronic devices which are sensitive to the nature of interface.

Interfacial intermixing across the interfaces at room temperature (RT) can change chemical states of the constituent elements which could play a crucial role and affect the electronic, magnetic and transport properties. X-ray photoelectron spectroscopy (XPS) is a unique surface sensitive technique, used to characterize the surface chemical compositions, electronic states and to probe the interfacial region of such structures [7].

Thus, motivation behind the present study is to investigate the presence of surface chemical states/chemical phases across Co_2FeAl/n-Si interface which might play a crucial role in magnetic and magnetotransport measurements across the interface. In this report, detailed analysis of XPS has been done. XPS spectra have shown the presence of metallic phases of Fe, Co and Al along with the signal due to Si substrates. Formation of various phases of silicides which were present in the XRD data of Fe/Co was also observed [1] and found to affect the magnetic and transport properties across the junction.

---

[*] E-mail: bhuarvind2512@gmail.com

2. Experimental

To realize the Co_2FeAl/n-Si interfacial structure, a thin film of Co_2FeAl (of ~50 nm thickness) has been deposited on etched and cleaned n-Si substrates by electron beam evaporation technique under the base pressure of ~1.33× 10^{-4} Pa.

XPS measurement was performed using VSW-ESCA photoelectron spectrometer at a base pressure of ~1.33 × 10^{-7} Pa at room temperature with AlKα X-rays (energy, hυ ~1486.6 eV) source. Hemispherical energy analyzer was used in the fixed analyzer transmission mode with the pass energy (~40 eV) to give an instrument resolution of ~0.9 eV. Other details regarding the metallization and XPS measurement have been given in our previous reports [1, 8, 9].

3. Results and discussion

3.1. Core level XPS study of Co_2FeAl/n-Si interfacial structure

Survey scan spectrum of Co_2FeAl films recorded over Si substrates is shown in Fig. 1. The survey scan spectrum contains photoemission peaks due to Fe, Co and Al at the binding energy (BE) positions of ~712.0 eV, ~779.7.0 eV and ~73.6 eV, respectively. Other peaks due to carbon (C), oxygen (O) and silicon (Si) have also been observed. The observed Si signal could be due to the interfacial intermixing across the interface. The presence of adsorbed impurities, such as carbon (C) and oxygen (O) signals detected on the sample's surface, could originate due to atmospheric exposure of the samples during the transfer to the chamber. To gain more insight about the interfacial chemistry, separate detailed scans for each element observed in the survey scan, i.e. for Co2p, Fe2p, Al2p and Si2p were also recorded. Furthermore, to analyze the variation in the content of Co, Fe and Al either in a form of silicide or oxide, the detail scan spectra of Co2p, Fe2p, Al2p and Si2p were further deconvoluted.

3.1.1. Detail scan spectrum of Co2p

A recorded core level XPS spectrum of Co2p peak is shown in Fig. 2 in a narrow scan between 820.0 eV and 760.0 eV. The recorded Co2p spectrum for as-deposited sample contains photoemission peaks due to $Co2p_{3/2}$ and $Co2p_{1/2}$ at binding energy positions of ~779.2 eV and 794.4 eV, respectively, which correspond to metallic phase of Co [10]. The difference between the observed doublet spectrum of Co2p is found to be of ~15.2 eV which is very close to the reported value of ~15.0 eV for metallic phase of Co [11, 12]. The peak at ~782.3 eV seems to correspond to Fe Auger peak or may be caused by the satellite peak of $Co2p_{3/2}$ [13] which also confirms the formation of the CFA alloy phase.

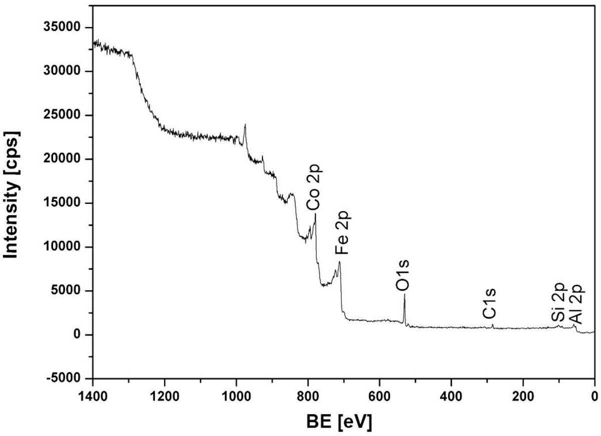

Fig. 1. Survey scan XPS spectrum of Co_2FeAl/n-Si interfacial structure.

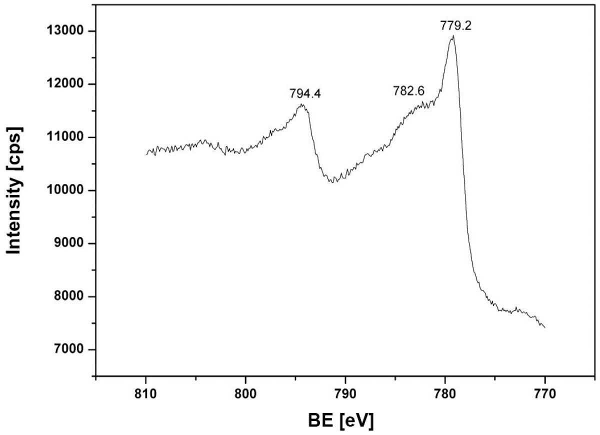

Fig. 2. Detail scan XPS spectrum of Co 2p of Co_2FeAl/n-Si interfacial structure.

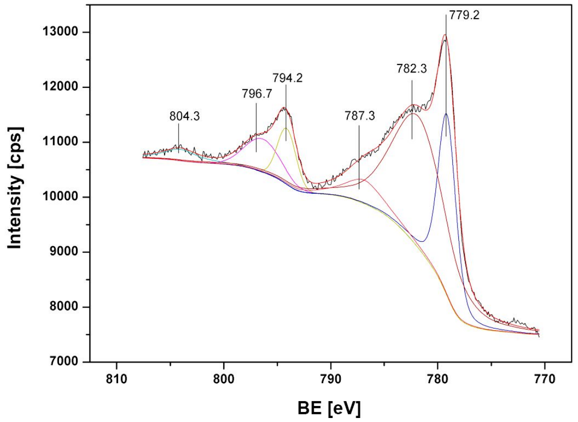

Fig. 3. Deconvoluted XPS spectrum of Co 2p of Co_2FeAl/n-Si interfacial structure.

3.1.2. Deconvoluted spectrum of Co2p

Fig. 3 shows the deconvoluted spectrum of Co2p for as-deposited sample. The spectrum of as-deposited sample has been deconvoluted into several peaks at BE positions of ∼779.2 eV, 782.3 eV, 787.3 eV, 794.2 eV and 796.7 eV. Peaks at binding energy positions of ∼779.2 eV (for $Co2p_{3/2}$) and 794.2 eV (for $Co2p_{1/2}$) are due to metallic phase of Co2p. Binding energy difference between Co2p doublet spectrum, i.e. Co $2p_{3/2}$ and $2p_{1/2}$ ∼15.0 eV is close to the standard separation between the doublet spectrum [12, 14]. The other observed peaks at binding energy positions of ∼782.3 eV and 796.7 eV show $Co2p_{3/2}$ and $2p_{1/2}$ spin-orbit doublet due to formation of Co-oxide phases (of CoO or Co_3O_4). Similar observation has also been reported by Tan et al. [15], where they found that the separation between spin-orbit doublet due to oxide phases of Co2p is ∼15.0 eV. The presence of shake-up satellite peak at BE ∼787.3 eV (∼5.0 eV higher than the $Co^{2+}2p_{3/2}$ ∼782.3 eV) could also be due to the oxide phase of cobalt (CoO/Co_3O_4). The observation of such shake up satellite peak ∼6.0 eV higher than $Co2p_{3/2}$ peak has also been reported in the literature [16]. Therefore, it seems that some trace amount of oxide phases are present along with the metallic phase of Co peak. The observed peaks of oxide phases can originate due to atmospheric exposure of the sample.

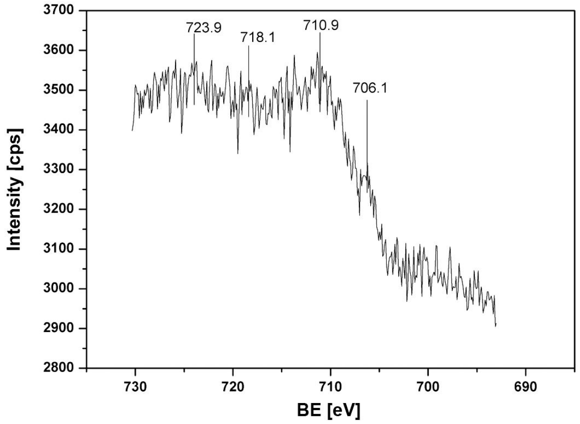

Fig. 4. Detail scan XPS spectrum of Fe 2p of Co_2FeAl/n-Si interfacial structure.

3.1.3. Detail scan spectrum of Fe2p

Fig. 4 shows the core level XPS spectrum of Fe2p peak for as-deposited sample, recorded in a narrow scan between ∼685.0 eV and ∼735.0 eV. The spectrum contains photoemission peaks of $Fe2p_{3/2}$ and $Fe2p_{1/2}$ at binding energy positions of ∼706.1 eV and 718.1 eV, respectively, which correspond to the metallic phase of iron. The other observed BE peaks positions at ∼710.9 eV and 723.9 eV seem to correspond to formation of iron silicide/oxide phase.

3.1.4. Deconvoluted spectrum of Fe2p

Fig. 5 shows the deconvoluted spectrum of Fe2p peak for an as-deposited sample. The spectrum has been deconvoluted into several peaks at BE positions of ∼706.1 eV, 710.9 eV, 719.2 eV and 723.9 eV. The peak positions at ∼706.1 eV ($Fe2p_{3/2}$) and 719.2 eV ($Fe2p_{1/2}$) correspond to the metallic phase of iron. The observed BE difference between Fe2p doublet spectrum, i.e. between $2p_{3/2}$ and $2p_{1/2}$ is 13.1 eV is close to the reported value [17]. The other observed BE peak positions at ∼710.9 eV ($Fe2p_{3/2}$) and 723.9 eV ($Fe2p_{1/2}$) seem to correspond to formation of iron silicide ($Fe_3Si/FeSi_2$) phase [18] or result from the formation of iron oxide phase. Such phase formation of iron has also been reported in the literature [19, 20]. It is also clear from the survey scan spectrum (Fig. 1) which shows the trace of Si signal which is likely to originate due to interfacial intermixing between Co_2FeAl alloy and Si substrate. The presence of such iron silicide phases has earlier been observed in our XRD data [1] which is now confirmed by our XPS data. The formation of such silicide phases could also result due to the strong chemical reactivity of n-type Si substrate [21].

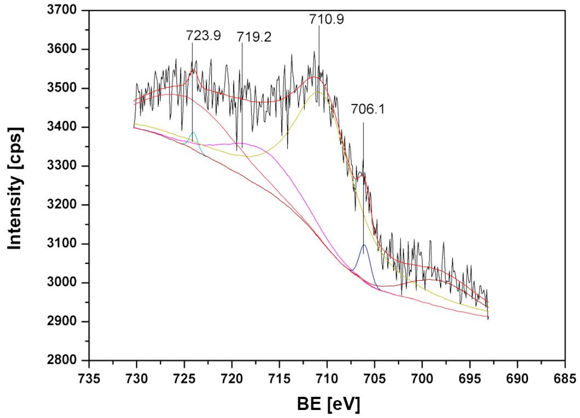

Fig. 5. Deconvoluted XPS spectrum of Fe 2p of Co_2FeAl/n-Si interfacial structure.

3.1.5. Detail scan spectrum of Al2p

Fig. 6 shows the core level XPS spectrum of Al2p peak recorded in a narrow scan between 85.0 eV and 65.0 eV. The recorded detail scan spectrum of Al2p shows the BE peak position at ∼73.6 eV which corresponds to presence of Al.

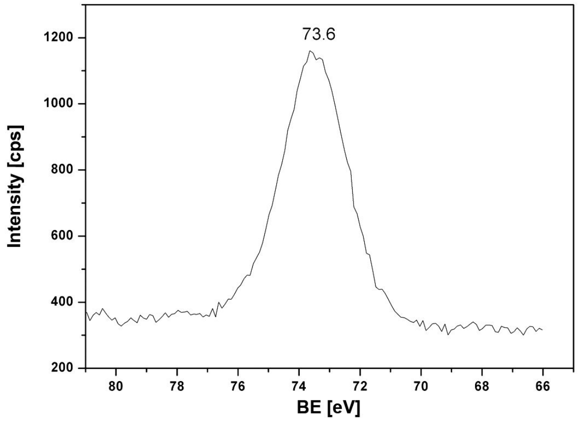

Fig. 6. Detail scan XPS spectrum of Al 2p of Co_2FeAl/n-Si interfacial structure.

3.1.6. Deconvoluted spectrum of Al2p

Fig. 7 shows the deconvoluted spectrum of Al2p signal. The spectrum shows the peak at BE position of ∼73.4 eV which corresponds to Al.

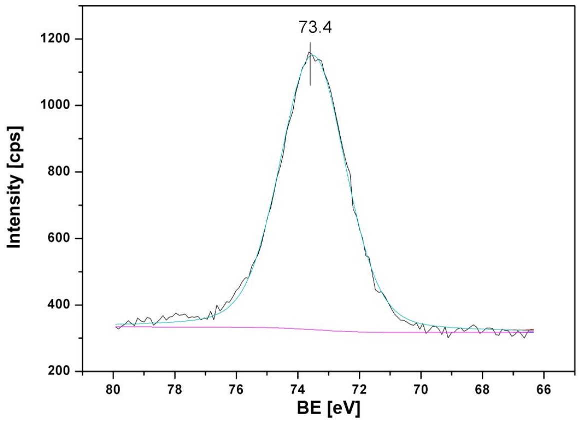

Fig. 7. Deconvoluted XPS spectra of Al 2p of Co_2FeAl/n-Si interfacial structure.

3.1.7. Detail scan spectrum of Si2p

Fig. 8 shows the core level XPS spectrum of Si2p peak recorded in a narrow scan between 120.0 eV and 90.0 eV. The recorded detail scan spectrum of Si2p shows the BE peak position at ∼100.8 eV which corresponds to the presence of Si Almand. (∼101.8 eV) or oxide phase [22].

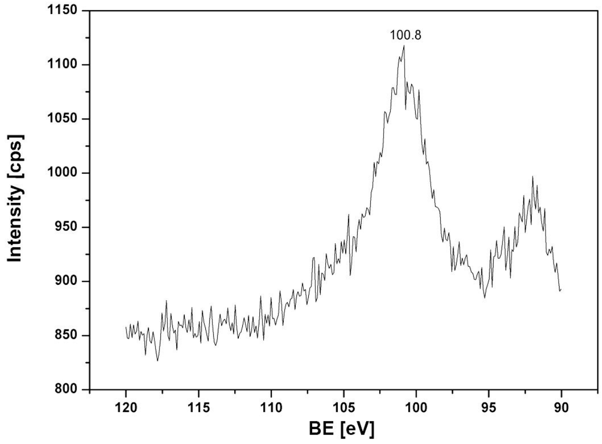

Fig. 8. Detail scan XPS spectrum of Si 2p of Co_2FeAl/n-Si interfacial structure.

3.1.8. Deconvoluted spectrum of Si2p

Fig. 9 shows the deconvoluted spectrum of Si2p signal. The spectrum shows the peak at BE position of ~100.1 eV corresponding to Si Almand. (~101.8 eV).

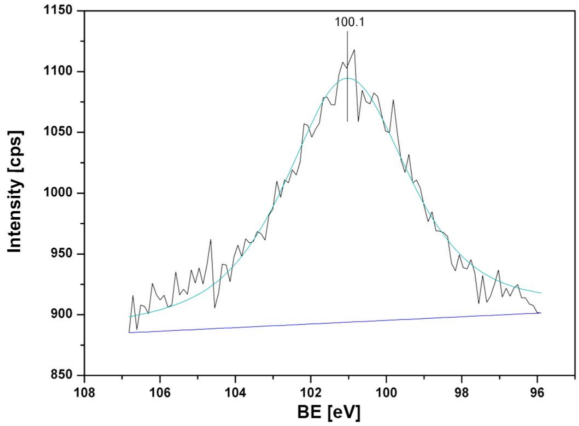

Fig. 9. Deconvoluted XPS spectra of Si 2p of Co$_2$FeAl/n-Si interfacial structure.

Thus, our present XPS study shows the presence of different chemical phases due to interfacial reactivity across the interfaces. The observed phases of Co, Fe and Al confirm the formation of CFA alloy phase. Other observed silicides (Fe$_3$Si/FeSi$_2$) and metallic iron phases in our XPS results can be understood due to the interfacial intermixing at the Co$_2$FeAl/Si interface. Si signal present in the XPS survey scan spectra supports the formation of silicide phases.

4. Conclusions

The role of interfacial chemistry modifications was studied using XPS technique to see its effect on transport and magnetic properties. It has been observed that there is a peak shifting in the BE positions of the Fe2p and Co2p peaks which has been explained by interfacial intermixing between the alloy and Si substrate resulting in phases formation, such as silicides and oxides. Formation of silicide phases due to interfacial intermixing could be due to the strong chemical reactivity of n-Si substrate. The presence of Si signal has confirmed the role of interfacial intermixing across the interface. Such interactions seem to be responsible for the electronic and magnetic properties of layered structures. Our present XPS investigations support our earlier study [1] on Co$_2$FeAl/n-Si interfacial structure.

Acknowledgements

We would like to thank Dr. U.P. Deshpande for his help and cooperation in the XPS measurements. Arvind Kumar also acknowledges the financial support received from the University Grants Commission, New Delhi, India, in the form of Senior Research Fellowship (UGC-SRF).

References

[1] Kumar A., Srivastava P.C., *J. Mater Sci.-Mater. El.,* 26 (2015), 5611.
[2] Rozale H., Lakdja A., Amar A., Chahed A., Benhelal O., *Comput. Mat. Sci.,* 69 (2013), 229.
[3] Galanakis I., Dederichs P.H. (Eds.), *Half-Metallic Alloys,* Springer, Berlin, 2005.
[4] Hirohata A., Kikuchi M., Tezuka N., Inomata K., Claydon J.S., Xu Y.B., Laan van der G., *Curr. Opin. Solid St. M. Sci.,* 10 (2006), 93.
[5] Li X.Q., Xu X.G., Zhang D., Miao J., Zhan Q., Jalil M.B.A., Yu G.H., Jiang Y., *Appl. Phys. Lett.,* 96 (2010), 142505
[6] Farshchi R., Ramsteiner M., *J.Appl. Phys.*, 113 (2013), 191101.
[7] Yamashita T., Hayes P., *Appl. Surf. Sci.,* 254 (2008), 2441.
[8] Kumar A., Shripathi T., Srivastava P.C., *J. Sci. Adv. Mat. Dev.,* 1 (2016), 290.
[9] Kumar A., Srivastava P.C., *J. Electron. Mater.,* 43 (2014), 381.
[10] Naik S.R., Rai S., Lodha G.S., Brajpuriya R., *J. Appl. Phys.,* 100 (2006), 013514.
[11] Li B., Ji M., Wu J., *J. Appl. Phys.,* 68 (1990), 1099.
[12] Galtayries A., Grimblot J., *J. Electron. Spectrosc.,* 98 (1999), 267.
[13] Ruhrnschopf K., Borgmann D., Wedler G., *Thin Solid Films,* 280 (1996), 171.
[14] Hassan S.S.A., Xu Y., Hirohata A., Sukegawa H., Wang W., Inomata K., Laan G.V., *J. Appl. Phys.,* 107 (2010), 103919.
[15] Tan B.J., Klabunde K.J., Sherwood P.M.A., *J. Am. Chem. Soc.,* 113 (1991), 855.
[16] Laureti S., Agostinelli E., Scavia G., Varvaro G., Albertini V.R., Generosi A., Paci B., Mezzi A., Kaciulis S., *Appl. Surf. Sci.,* 254 (2008), 5111.
[17] Barbieri A., Weiss W., Hove M.A.V., Somorjai G.A., *Surf. Sci.,* 302 (1994), 259.
[18] Ohtsu N., Oku M., Satoh K., Wagatsuma K., *Appl. Surf. Sci.,* 264 (2013), 219.
[19] Hong S., Wetzel P., Gewinner G., Bolmont D., Pirri C., *J. Appl. Phys.,* 78 (1995), 5404.

[20] EGERT B., PANZNER G., *Phys. Rev. B*, 29 (1984), 2091.
[21] GARRISON B.J., GODDAID W.A., *Phys. Rev. B*, 36 (1987), 9805.
[22] SRIVASTAVA N., SRIVASTAVA P.C., *J. Electron. Spectrosc.,* 191 (2013), 20.

Received 2018-03-29
Accepted 2018-07-25