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Studies on the valence electronic structure of Fe and Ni in Fe_xNi_{1-x} alloys

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Abstract. K_β-to-K_α X-ray intensity ratios of Fe and Ni in pure metals and in Fe_xNi_{1-x} alloys ($x = 0.20$, 0.50, 0.58) exhibiting similar crystalline structure have been measured following excitation by 59.54 keV γ-rays from a ^{241}Am point source, to understand as to why the properties of permalloy $Fe_{0.2}Ni_{0.8}$ is distinct from other alloy compositions. It is observed that the valence electronic structure of $Fe_{0.2}Ni_{0.8}$ alloy is totally different from other alloys which may be attributed to its special magnetic properties.

Keywords. K_β-to-K_α ratio; alloy; valence electronic structure.

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1. Introduction

Fe_xNi_{1-x} alloys have emerged as technologically important materials due to the rapid advance of magnetoelectronics [1]. Although the studied Fe_xNi_{1-x} alloys ($x = 0.2$, 0.5 and 0.58) crystallize in the same γ (fcc) phase, permalloy, a member of the family of Fe_xNi_{1-x} alloys (with $x = 0.2$), exhibits distinct physical properties of vanishingly small magnetostriction, low coercivity and high permeability, which makes it the material of choice for magnetic recording media, sensors and non-volatile magnetic random access memory. Accordingly, it is very important to have a detailed knowledge of the valence electronic structure of Fe and Ni in various Fe_xNi_{1-x} alloys. Since K_β-to-K_α X-ray intensity ratio has been reported [2–7] to be a sensitive physical parameter to investigate the changes in the valence electronic structure of $3d$-transition metals [2], we have undertaken the study of the valence electronic structure of Fe and Ni in the Fe_xNi_{1-x} alloys for various compositions ($x = 0.2$, 0.5 and 0.58) exhibiting similar crystalline structure to understand as to why the physical properties of $Fe_{0.2}Ni_{0.8}$ alloy are drastically different from other alloy compositions. The important results of the study are reported here while the details have been communicated elsewhere [7].

2. Experiment

The measurements were carried out using high purity alloys (in powder form) procured from Alpha, a Johonson Mathey Company, UK. The powder material is pelletized and 59.54 keV γ-rays from a 200 mCi ^{241}Am point-source were made to incident on the pellet to ionize the target atoms. The emitted X-rays were detected and were finally recorded in a Canberra PC based Model S-100 multichannel analyzer. The X-ray spectra thus obtained were carefully analyzed with the help of a multi-Gaussian least-square fitting programme [8] using a non-linear background subtraction. Details regarding the experimental arrangement as well as data analysis have been reported elsewhere [3,4,7].

3. Results and discussion

The experimental results for the K_β-to-K_α X-ray intensity ratios of Fe and Ni in pure metals and in the $\mathrm{Fe}_x\mathrm{Ni}_{1-x}$ alloys ($x = 0.2$, 0.5 and 0.58) before and after various corrections are presented in table 1. The errors quoted in the table are only statistical. The $3d$ electron populations of Fe and Ni for various samples are presented in table 2. These have been

Table 1. Experimental K_β/K_α X-ray intensity ratios for Fe and Ni in $\mathrm{Fe}_x\mathrm{Ni}_{1-x}$ alloys.

	K_β-to-K_α ratio of Fe		K_β-to-K_α ratio of Ni	
Composition (x)	Before correction	After correction	Before correction	After correction
0	—	—	0.1808 ± 0.0016	0.1346 ± 0.0012
0.2	0.1737 ± 0.0010	0.1326 ± 0.0008	0.1723 ± 0.0010	0.1314 ± 0.0008
0.5	0.1743 ± 0.0009	0.1321 ± 0.0007	0.1808 ± 0.0010	0.1371 ± 0.0008
0.58	0.1726 ± 0.0008	0.1309 ± 0.0006	0.1822 ± 0.0010	0.1386 ± 0.0008
1.0	0.1764 ± 0.0009	0.1307 ± 0.0007	—	—

Table 2. Evaluated $3d$-electron population values and total number of ($4s$, $4p$) electrons for Fe and Ni in various samples.

Kind of sample	Evaluated $3d$-electron population for Fe	Total number of ($4s, 4p$) electrons for Fe	Evaluated $3d$-electron population for Ni	Total number of ($4s, 4p$) electrons for Ni
Pure Fe	7.39 ± 0.29	0.61 ± 0.29	—	—
Pure Ni	—	—	8.54 ± 0.39	1.46 ± 0.39
$\mathrm{Fe}_{0.2}\mathrm{Ni}_{0.8}$	6.69 ± 0.26	1.31 ± 0.26	9.93 ± 0.52	0.07 ± 0.52
$\mathrm{Fe}_{0.5}\mathrm{Ni}_{0.5}$	6.86 ± 0.24	1.14 ± 0.24	7.81 ± 0.21	2.19 ± 0.21
$\mathrm{Fe}_{0.58}\mathrm{Ni}_{0.42}$	7.31 ± 0.24	0.69 ± 0.24	7.44 ± 0.19	2.56 ± 0.19

Table 3. Comparison of estimated weighted average number of 3*d* and (4*s*, 4*p*) electrons for various Fe_xNi_{1-x} alloys with the superposition values of 3*d* and (4*s*, 4*p*) electrons obtained from the pure metal values.

Kind of sample	Weighted average number of 3*d* electrons	Superposition of 3*d* electrons obtained from pure metal values	Weighted average number of (4*s*, 4*p*) electrons	Superposition of (4*s*, 4*p*) electrons from pure metal values
$Fe_{0.2}Ni_{0.8}$	9.28 ± 0.42	8.31 ± 0.32	0.32 ± 0.42	1.29 ± 0.32
$Fe_{0.5}Ni_{0.5}$	7.34 ± 0.16	7.97 ± 0.24	1.66 ± 0.16	1.03 ± 0.24
$Fe_{0.58}Ni_{0.42}$	7.36 ± 0.16	7.87 ± 0.24	1.48 ± 0.16	0.97 ± 0.24

evaluated by comparing the experimental values of K_β-to-K_α intensity ratio with the results of MCDF calculations performed for various valence electronic configurations [2] of Fe and Ni. The 3*d* electron populations, thus obtained, for pure Fe and Ni metals (table 2) are found to be in close agreement with the results of band structure calculations of Papaconstantopoulos [9] (6.93 for Fe and 8.97 for Ni) and Hodges *et al* [10] (8.82 for Ni). In order to answer as to why the physical properties of $Fe_{0.2}Ni_{0.8}$ alloy are distinct as compared to the other two alloys, we have calculated the *weighted average* numbers of 3*d* and (4*s*, 4*p*) electrons per one atom as well as the superposition of 3*d* and (4*s*, 4*p*) electrons, as obtained from pure metal values, for all the studied Fe_xNi_{1-x} alloys and the results are shown in table 3. It can be seen from table 3 that in the case of $x=0.5$ and 0.58 the weighted average numbers of 3*d* electrons in the Fe_xNi_{1-x} alloys (the second column of table 3) are smaller than the superpositions of the number of 3*d* electrons of pure Fe and Ni metals (the third column of table 3). In the case of $Fe_{0.2}Ni_{0.8}$ alloy the weighted average number of 3*d* electrons is very large (9.28 ± 0.42) and differs considerably from the superposition of the number of 3*d* electrons of pure Fe and Ni metals (8.31 ± 0.32). However, in the case of (4*s*, 4*p*) electrons the situation is opposite. Clearly, there is considerable difference of the valence electronic structure of $Fe_{0.2}Ni_{0.8}$ alloy with respect to the other two alloys.

4. Conclusion

The study of K_β-to-K_α intensity ratio along with the MCDF calculation reveals a large weighted average number of 3*d* electrons (9.28 ± 0.42) and negligible weighted average number of (4*s*, 4*p*) electrons (0.32 ± 0.42) for $Fe_{0.2}Ni_{0.8}$ alloy as compared to other studied alloys. The considerable difference in the valence electronic structure of $Fe_{0.2}Ni_{0.8}$ alloy may possibly be the reason for the high permeability and other alluring magnetic properties of this alloy.

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