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A XAFS Study on the Site Determination of Additives in the Ni₃Al Intermetallic Compound

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Abstract. Occupied sites by dopants of Ag(0.1at%), Pd(2at%) and Zr(0.4at%) in the Ni₃Al intermetallic compound are investigated by means of EXAFS analysis. It is found that Pd substitutes the Ni site and Zr substitutes the Al site. These results are consistent with those of channeling enhanced microanalysis. Ag is also determined to substitute in the Ni site by EXAFS and this result supports that Ag additive is γ -phase(disorder phase) former. The expansion of the nearest neighbor distance around Ag, Pd, and Zr are 2%, 3% and 4% respectively.

1. INTRODUCTION

Ni₃Al intermetallic compound having the L1₂ ordered structure is well known as a high temperature material. Lack of ductility of this Ni₃Al compound, however, restricts the application. To improve their ductility it has been found that the addition of the third elements are effective[1]. Chiba et. al. have found by channeling enhanced microanalysis that Pd has a strong tendency to substitute a Ni site independent of the composition of the host alloy. Furthermore, they have discovered that Ag also improves the ductility of the Ni₃Al compound. There are no experimental results, however, which site Ag substitutes in the Ni₃Al because of experimental difficulty due to a small amount of Ag content(<0.1at%). The aim of this study is to determine the occupied site of the dilute dopants of Ag, Pd and Zr in the Ni₃Al by means of EXAFS and discuss about the lattice expansion around doping atoms.

2. EXPERIMENTAL

Three different doped Ni₃Al samples were prepared: 0.1at%Ag, 2at%Pd and 0.4at%Zr. The XAFS spectra of Pd, Zr and Ag K-edge were obtained at the beam line BL6B of KEK Photon Factory with 3GeV operation mode. Fluorescence X-ray detection mode was applied for all specimens with using SSD as an X-ray detector to eliminate background signal due to elastic scattering and fluorescence X-rays emitted from Ni. Fe Filter was inserted in between the sample and the detector to minimize fluorescence X-rays emitted from Ni. All measurements have been done at room temperature and ring current was 120 - 190mA. The X-ray energy was defined by a Si(311) double crystal monochromator with sagittal focusing.

3. RESULTS AND DISCUSSION

Fourier transform ($F(r)$) of the Ag K-edge EXAFS for Ni₃Al-0.1at%Ag, the Pd K-edge EXAFS for Ni₃Al-2at%Pd and the Zr K-edge EXAFS for Ni₃Al-0.4at%Zr are shown in Fig.1. Fourier transformations are done on the k range of $3.5 - 12.5\text{\AA}^{-1}$ for the Ag K-edge EXAFS and $3.5 - 16\text{\AA}^{-1}$ for the Pd and the Zr K-edge EXAFS. It should be noted that $F(r)$'s of Ag and Pd EXAFS show a small peak around $3.2\text{\AA}$ (pointed by the arrow in the figure). On the other hand, there are no peaks at this position in the $F(r)$ for Zr EXAFS. Chiba et. al. have reported that Pd has a strong tendency to substitute a Ni site while Zr substitute a Al site from channeling enhanced microanalysis[1]. By taking into account the results of the channeling enhanced microanalysis, it is obvious that the peak located at $3.2\text{\AA}$ in the $F(r)$ is characteristic for Ni site in the Ni₃Al intermetallic compound. The second shell around Ni site in the Ni₃Al compound consists of 6 Ni atoms with distance of $3.56\text{\AA}$, while that around Al site has 6 Al atoms with the same distance. Since an Al atom has small back scattering amplitude, it can be said that the peak corresponding to the second shell around Al site should be weak.

The differences in the $F(r)$ between Ni and Al sites in the Ni₃Al compound are examined by theoretical calculation. Theoretical EXAFS calculations was carried out by applying program FEFF6[2] for the model structures of Ag, Pd and Zr atoms substitute Ni or Al site in the Ni₃Al intermetallic compound. As shown in Fig. 2, there is a peak at $3.2\text{\AA}$ in the $F(r)$ for all the elements substituting the Ni site while no peak exists at $3.2\text{\AA}$ for all elements substituting the Al site. The distance of the first shell around Ni in ordered Ni₃Al is $2.52\text{\AA}$ and that of the second shell is $3.56\text{\AA}$ for both of the Ni site and the Al site.

Figure 1: Magnitude of the Fourier transform $F(r)$ for EXAFS of 0.1at%Ag, 2at%Pd and 0.4at%Zr dopants in the Ni_3Al compound. See details in text.

Figure 2: Magnitude of the Fourier transform $F(r)$ for EXAFS calculated by FEFF6[2] around Ag, Pd and Zr dopants in the Ni_3Al compound with L12 structure. Substitute sites of these dopants are indicated in the figure.

However, these theoretical calculations show no peaks at around $3.2\text{\AA}$ for the Al site same as experimental results. Therefore this second correlation peak at $3.2\text{\AA}$ in the $F(r)$ is characteristic for the dopants occupying the Ni site. Chiba et al. suggested that the ternary elements decreasing the ordering energy tend to substitute the Ni site while the elements increasing the ordering energy tend to substitute the Al site[3]. According to this classification, Ag and Pd substitute the Ni site and Zr substitute the Al site[3]. The experimental results of EXAFS for Ag, Pd and Zr dopants are consistent with these classification.

We use a simple substitution model in the FEFF calculation that atomic distances in the calculation are same as Ni_3Al compound. The positions of the first peak in the $F(r)$ calculated by FEFF are $2.16\text{\AA}$ for both of Pd and Ag dopants and $2.17\text{\AA}$ for Zr. On the other hand, experimental results show the position of the first peak at $2.21\text{\AA}$ for Ag, $2.23\text{\AA}$ for Pd and $2.26\text{\AA}$ for Zr. These results suggest that the dopants investigated in the present study give some stresses to Ni_3Al lattice. The estimated expansion of the distance of the first nearest correlations are 2% for Ag, 3% for Pd and 4% for Zr. The atomic radii of Ni and Al are 1.24 and $1.43\text{\AA}$ respectively, while those of Ag, Pd and Zr are 1.44 , 1.37 and $1.60\text{\AA}$. Therefore, all dopants have possibility to cause local lattice expansion. This is the first experimental observation about the expansion of the atomic distance caused by the dopant. It is still not clear, however, whether this lattice expansion is associated the ductility improvement.

In this system, degree of chemical ordering around doped atoms is important to discuss about the stability of ordered phase. The curve fitting results shows that the coordination number of Al and Ni around Pd atom are 5.0 ± 0.5 and 7.0 ± 0.5 respectively and that around Ag are 4.3 ± 0.5 and 7.7 ± 0.5 respectively. On the other hand, the first shell around Ni site is occupied by 4 Al atoms and 8 Ni atoms in the Ni_3Al compound. This higher coordination number of Al around Pd atom obtained from EXAFS is supported by the higher bonding strength of Pd-Al than Pd-Ni[4]. Consequently, it can be concluded that Pd dopant tend to cause chemical disorder in the Ni_3Al compound. The case of Zr dopant, EXAFS results shows that Zr atom is surrounded by 12 Ni atoms then same as the local structure around Al site.

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