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ALCHEMI OF Fe-DOPED B2-ORDERED NiAl ALLOYS WITH DIFFERENT DOPING LEVELS

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Recently, a formulation of the ALCHEMI technique¹ has been presented² that yields exact expressions for best-fit parameters^{3,4} in terms of the ionization localization constants and site distributions of three elements distributed over two sublattices. The application of this formulation to a NiAl-based B2-ordered alloy doped with 10% Fe used a graphical plotting technique⁵ to show that the size of the standard error of the best-fit parameters (and therefore of the site distributions) correlates with the extent to which the plotted data define a unique plane. The definition of the plane depends both upon the scatter of the data (Poisson statistics) and the spread of data over the best-fit plane (the variety of channeling conditions sampled). In this paper, the graphical plotting technique is applied to Fe-doped NiAl B2-ordered alloys of composition $\text{Ni}_{0.5-x}\text{Fe}_x\text{Al}_{0.5}$ with $x \in \{0.02, 0.10\}$.

Thin foil specimens of each composition were examined in a Philips CM12 operated at 120 kV and equipped with an EDAX 9900 ultra-thin window energy-dispersive X-ray spectrometer. Numerous spectra were acquired from a single area of the specimen. During acquisition of each data set, the diffracting conditions were varied by tilting the electron beam using the dark-field deflectors; in this way, the geometry of the specimen relative to the X-ray detector was fixed so that the absorption of Al-K X rays would be the same for all spectra. The intensities of the characteristic peaks, $I_i(k)$, of each element, i , in each spectrum (k) are normalized to the intensities, $I_i(0)$, recorded in a weakly channeling ("random") orientation. The resulting ratio of intensities, $r_i(k)$, is a measure of the channeling effect for element i at the orientation for which spectrum (k) was acquired. If the channeling is dominated by a single set of crystallographic planes,⁶ the normalized intensities $r(k) = (r_{\text{Ni}}(k), r_{\text{Al}}(k), r_{\text{Fe}}(k))$ should lie in a plane. Mathematica™ has been used to plot the data from two complementary perspectives perpendicular to the r_{Fe} axis: (a) in the best-fit plane of the data and (b) at 90° to the first.

Plots of the data for the specimens with 2% and 10% Fe doping levels are shown in Figures 1 and 2, respectively. The two figures are not of the same scale; Figs. 1b and 2b are of similar projected area when the figures are drawn at the same scale. The vertical axes of all plots are parallel to the r_{Fe} -axis. The orientation of the horizontal axis depends upon the relative size of the best-fit parameters. The horizontal axes in Fig. 1 and 2 are approximately parallel to the r_{Ni} -axis in (a) and to the r_{Al} -axis in (b). The data from the 2% alloy were acquired under planar channeling conditions at the (200) systematic; the data from the 10% alloy were acquired under axial channeling conditions at the [001] pole. Table I gives the corresponding best-fit parameters, α_i , and the inferred site occupancies. Since for both alloys the Fe resides almost exclusively on the 'Ni'-site, the effect of constitutional point-defects (vacancies or anti-sites) on the results is negligible.^{2,5} One-sigma error bars are quoted for all parameters extracted from the fit. The error bars do not reflect a systematic error that may arise from an erroneous choice of the weakly channeling intensities, $I(0)$, used to normalize the $r(k)$.

Figs. 1a and 2a show that the r_{Fe} and r_{Ni} axes are similar in dimension, reflecting a common site distribution and similar localization constants (≈ 1) of the Fe and Ni atoms. However, because the electron intensity is preferentially channeled onto the 'Ni'-sites at the (200) systematic orientation, the dimension of the r_{Al} -axis is considerably smaller than that of the r_{Fe} - and r_{Ni} -axes in Fig. 1. Conversely, the r_{Al} -axis is of larger dimension relative to the r_{Fe} - and r_{Ni} -axes in Fig. 2 because the electron intensity is preferentially channeled onto the 'Al'-sites at the [001] pole. If the magnitude of the channeling effect on the 'Ni' and 'Al' sites were similar, the r_{Al} -axis would be of smaller dimension than the r_{Ni} axis in proportion with the localization constants for Al and Ni.

The average number of counts recorded in the Fe- K_{α} peaks of the spectra are ~ 1300 for the 2% alloy and $\sim 10,000$ for the 10% alloy. The relative statistical error, which varies as $1/\sqrt{N}$, is therefore almost three times greater for the 2% alloy. The poorer Poisson statistics are reflected in the greater scatter of the data in Fig. 1a relative to that in Fig. 2a. However, the spread of the data within the best-fit plane is better for the 2% alloy (Fig. 1b) than for the 10% alloy, for which the data is spread nearly linearly (Fig. 2b). The standard error of the 2% alloy is correspondingly better than that of the 10% alloy (Table I), in spite of the poorer counting statistics.⁷

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Table I: Results of ALCHEMI analysis of Fe-containing NiAl.

Specimen	pole or planes	Best-fit Parameters		Fraction of Fe on 'Ni' site $p_{\text{Fe:Ni}}$ (%)
		α_{Ni}	α_{Al}	
2% Fe ($\text{Ni}_{0.48}\text{Fe}_{0.02}\text{Al}_{0.50}$)	(200)	0.968 ± 0.025	-0.021 ± 0.050	96.8 ± 2.5
10% Fe ($\text{Ni}_{0.40}\text{Fe}_{0.10}\text{Al}_{0.50}$)	[001]	0.946 ± 0.037	0.138 ± 0.018	94.6 ± 3.7

Figure 1: Plots of normalized intensities, $r^{(k)}$, from NiAl doped with 2% Fe ($\text{Ni}_{0.48}\text{Fe}_{0.02}\text{Al}_{0.50}$), viewed perpendicular to the r_{Fe} -axis (a) in the best-fit plane and (b) rotated 90° relative to (a).

Figure 2: Plots of normalized intensities, $r^{(k)}$, from NiAl doped with 10% Fe ($\text{Ni}_{0.40}\text{Fe}_{0.10}\text{Al}_{0.50}$), viewed perpendicular to the r_{Fe} -axis (a) in the best-fit plane and (b) rotated 90° relative to (a).

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