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Influence of Cr addition on the defect structure of Fe–Al alloys

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Abstract

The effect of 10 at% Cr addition to Fe-alloys containing 25 and 30 at% Al and the influence of the thermal treatment on the defect structure of these samples have been investigated by positron lifetime spectroscopy. Calculations have been performed to study the influence of Cr impurities on the lifetime associated to vacancy-type defects in both the $D0_3$ and B2 phases. The results show that Cr addition leads to a decrease of positron lifetime parameters associated with an increase of the $D0_3$ order.

Keywords: A. Ternary alloy systems; A. Iron aluminides, based on Fe_3Al; D. Defects: point defects; F. Spectroscopic methods, various

1. Introduction

The mechanical properties of the FeAl alloys can be improved with the addition of a third element. The magnitude of changes in these properties depends on many parameters such as the amount and type of the ternary element and the alloy composition, among others [1,2 and references therein]. Cr can improve the mechanical behaviour without affecting significantly the corrosion properties of the material. McKamey et al. [3] found that the room temperature ductility of Fe–Al alloys can be increased by partly substituting iron by chromium. Also, according to Klein and Baker [4] the addition of 5% chromium to the $Fe_{55}Al_{45}$ alloy significantly increases both yield and fracture strengths. More recently, the analysis performed by Palm [5] shows that Cr gives rise to solution hardening in alloys containing about 26% Al. Particularly, the knowledge of the Cr site preference is very important to understand the changes in the mechanical behaviour of the ternary alloys. It has been found by using theoretical [6–9] and experimental [10,11] techniques that Cr atoms prefer Al sites in B2 Fe–Al alloys. However, Munroe and Kong [2] have determined that Cr atoms evenly occupy substitutional sites in both, Fe and Al sublattices for the $Fe_{45}Al_{50}Cr_5$ and $Fe_{49}Al_{50}Cr_1$ alloys. Anderson [12] has obtained additional evidence indicating the possibility of Cr substitutions also in the Fe sublattice of B2 Fe–Al alloys. On the other hand, Kim and Morris examined Cr site location for Al-rich Fe_3Al(Cr) annealed to both B2 and $D0_3$ orders [13]. These authors deduced from the value of the long range order parameter determined from neutron powder diffraction measurements that in B2 ordering Cr atom prefers to locate on Al sublattice and on Fe(1) site (4(b) sites in Wickoff notation) of $D0_3$ ordered alloy.

Several studies have demonstrated that the mechanical properties of Fe–Al alloys are highly influenced by the presence of vacancies retained in the lattice following heat treatments at elevated temperatures [1,2 and references therein, 14]. It is expected that the vacancy–ternary atom interaction will play an important role in the mechanical properties of the Fe–Al based ternary alloys. Owing to the high sensitivity of positrons to open-volume defects, the positron annihilation spectroscopy is a valuable technique to study vacancy-type defects and interactions with impurities [15,16]. Previous

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works have demonstrated the utility of this technique to study the Fe–Al system [17–21]. In this work the positron lifetime technique is used to investigate the behaviour of vacancies in different Fe–Al–Cr alloys as a function of both composition and cooling rate. The experimental data are complemented by lifetime calculations.

2. Experimental procedure and results

Two ternary and two binary alloys, whose chemical composition is shown in Table 1, were prepared in the Max-Planck-Institut für Eisenforschung (Düsseldorf). Iron, aluminium and chromium with a purity of 99.98, 99.9995 and 99.95%, respectively, were used. The alloys were induction melted in alumina crucibles and cast into ingots under a pressure of 40 kPa of high purity argon. Three sets of samples from each composition were annealed in air at 1000 °C for 2 h. In order to ensure a different content of retained defects, all compositions were given three different treatments as follows:

(a) Air quenching (AQ samples).
(b) Slow furnace cooling down to room temperature (FC samples). It took 8 h to cool down to 100 °C.
(c) Air quenching followed by ageing at 410 °C during one month and slow furnace cooling at a rate of 13 K/day (MA samples).

For the positron lifetime measurements a fast system with a resolution of 230 ps was used and a conventional ^{22}Na source on a Kapton foil was employed as a positron source. A constant component of 380 ps with 13.5% intensity was present in all the samples and was subtracted to all the spectra as the source contribution. After the source subtraction, the spectra were analysed satisfactorily with three or two components. From these, the longest had a value of about 2 ns with a very faint intensity and was roughly constant, irrespective of the sample and thermal treatment. Thus, it was concluded that this long lifetime is not characteristic of the defect state of the alloy and will not be considered in further discussions.

The results of the positron lifetime measurements are summarised in Fig. 1 for all the studied alloys and conditions; in the graphs the average lifetimes are plotted for each thermal treatment. Each point is the average of three measurements and the error bars for the average lifetime $\overline{\tau}$ are equal or smaller than the symbol size and, therefore, they are not shown in the figure. The values in the boxes correspond to the results of the two-component spectra and denote the lifetimes associated to defects (τ_d) and their relative intensities (I_d).

Table 1
Composition of the investigated alloys

Alloy	Composition (at%)		
	Fe	Al	Cr
A	65	25	10
B	75	25	–
C	60	30	10
D	70	30	–

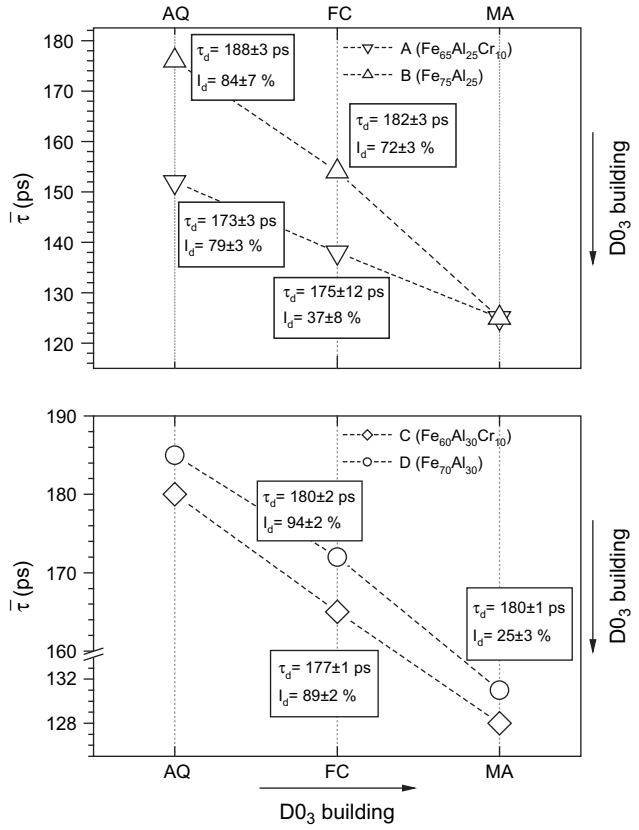

Fig. 1. The positron annihilation parameters as a function of the thermal treatment. The error bars for the average lifetime $\overline{\tau}$ are equal or smaller than the symbol size. The figures in the boxes denote the values of the second component τ_d and its associated intensity I_d for the two-component spectra.

3. Lifetime calculations

Several types of defects involving vacancies and substitutional Cr atoms have been studied. Only the vacancy-type defects relevant for the $D0_3$ and B2 structures in the Fe–Al system have been considered. According to a recent study [21], these are triple defects (TD) and monovacancies in the B2 phase. The former are present at high temperature and are described as a complex, in which two adjacent Fe vacancies in the ⟨100⟩ direction are bound to a Fe atom on an Al site in the nearest neighbour position. Recently Nogueira and Schön [22] have predicted that the triple defect is metastable and must be destroyed during diffusion in good agreement with our experimental results [21]. The low temperature vacancy-type defect can be described as an unbound TD in which the two vacancies are far from the antisite and can be identified as monovacancies in the Fe sublattice. Monovacancies in the $D0_3$ structure are only observed at high temperatures. For the monovacancies in the $D0_3$ and B2 states only the case of a Cr impurity in the nearest neighbour position has been investigated. For the Cr atom located in the vicinity of the TD several positions have been considered and shown in Fig. 2.

The positron lifetimes were calculated using the superimposed atom model of Puska and Nieminen [23]. Further details concerning these types of calculations have been given