



	Experiment title: Diffusion mechanism of iron in Ni ₄₀ Fe ₁₀ Al ₅₀ studied with forward scattering of synchrotron radiation	Experiment number: HS-1176
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Report:

B2 ordered intermetallics are considered as a basis for developing structural materials for high temperature applications [1]. The interest has aroused due to their unique physical and mechanical properties which has led to numerous important material developments. The common difficulties with intermetallics finding commercial applications are the poor ductility at room temperature and the problem of processing these materials inexpensively. In the last few years, however, considerable progress has been made in obtaining reproducible and technically interesting mechanical properties.

Ni-Al alloys have attracted a lot of attention due to their excellent properties, such as low density, high melting point, etc. However, they have not been utilised mainly due to the lack of room temperature ductility. Efforts to improve the ductility often include the addition of ternary or higher-order alloy components. The system NiAl with added Fe has received attention because of improved room-temperature ductility [2] and high-temperature creep properties. The site-occupation investigations [3] indicate that Fe tends to act as a buffer between the two sublattices, preferentially occupying the site of the stoichiometrically deficient host element. However, the Fe alloying addition was found to partition between the two sublattices to some extent, thus Ni-site vacancies or Ni anti-site defects are required to maintain the site balance.

The cylindrical single crystals of NiAl with about 20% of the Ni atoms replaced by Fe probe atoms was grown by the Bridgman method (according to microprobe fluorescence analysis: 49.0(2) at.% Al, 40.2(9) at.% Ni and 10.8(1.0) at.% Fe). The slices oriented with their surface normal to the [111] crystal axes were cut and mechanically polished to the thickness of about 30 µm for the nuclear forward scattering (NFS) experiment. Measurements were performed in a vacuum furnace. The spectra were taken between room temperature and 1500K (see Fig. 1, left) with the wave vector of synchrotron radiation parallel to the (113) crystal direction. Following the theory of Smirnov and Kohn [4] and our previous experiments [5], an accelerated decay rate Γ of the intensity decay at higher temperatures is caused by the diffusional jumps of iron atoms. Plotting Γ as

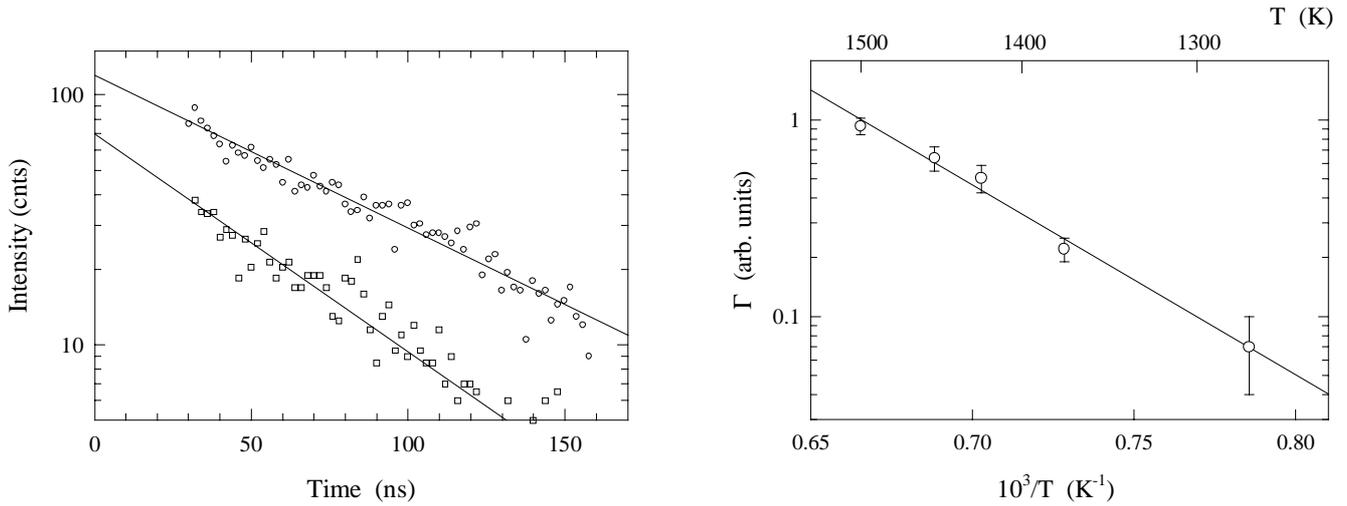


Fig. 1. (left) Nuclear forward scattering of SR from the (Ni,Fe)Al sample at 1270K (circles) and at 1500K (squares); (right) Arrhenius plot of the accelerated decay rate Γ in NFS spectra vs reciprocal temperature.

a function of temperature we can determine the value of the activation energy $Q = 1.8(3)$ eV for iron diffusion in the (Ni,Fe)Al alloy (see Fig 1, right). The activation energy for iron diffusion in Ni-Al is lower than this energy for nickel self-diffusion in the NiAl alloy of stoichiometric composition $Q = 3.01(4)$ eV due to the tracer measurements by Divinsky et al. [6].

The effect of much lower activation energy for iron diffusion than for Ni diffusion in Ni-Al confirms excellently the result of solid-solution hardening by Fe addition to Ni-Al by Pike et al. [7]. For the stoichiometric alloy (50 at.% Al atoms) the hardness was found to increase more rapidly with increasing Fe content than would be expected from the effect of the Fe defects alone. It is argued that this hardening could be attributed solely to the *increase in the vacancy concentration* that occurs with the addition of Fe.

The excess vacancies decrease the migration energy for Fe atoms and, assuming the same formation energy for Ni vacancies in the ternary alloy like in the binary NiAl (≈ 0.7 eV [8]), the resulting migration energy for Fe will be only 1.2 eV in place of 2.44 eV for Ni diffusion in NiAl.

The iron diffusion coefficient in (Ni,Fe)Al alloy calculated from our NFS measurement is about 2×10^{-14} $m^2 s^{-1}$ at 1500K and is almost 10 times larger than for the Ni diffusion in NiAl [6]. This result can also be explained with the increased vacancy concentration in the ternary phase in agreement with Ref. [7].

- [1] G. Sauthoff, *Intermetallics*, VCH Weinheim (1995).
- [2] R. Darolia, D.F. Lahrman and R.D. Field, *Scripta Metall Mater.* **26**, 220 (1992).
- [3] I.M. Anderson; A.J. Duncan and J. SO. Bentley, *Intermetallics* **7**, 1017 (1999).
- [4] G.V. Smirnov and V.G. Kohn, *Phys. Rev. B* **52**, 3356 (1995); V.G. Kohn and G.V. Smirnov, *Phys. Rev. B* **57**, 5788 (1998).
- [5] B. Sepiol, A. Meyer, G. Vogl, R. Ruffer, A.I Chumakov, A.Q.R. Baron, *Phys.Rev. Lett.* **76**, 3220 (1996); B. Sepiol, A. Meyer, G. Vogl, H. Franz, and R. Ruffer, *Phys. Rev. B* **57**, 10433 (1998).
- [6] S.V. Divinski, St. Frank, Chr. Herzig and U. Södervall, *Solid State Fenomena*, **72**, 203 (2000).
- [7] L.M. Pike, Y.A. Chang and C.T. Liu, *Intermetallics* **5**, 601 (1997).
- [8] S. Divinski and Chr. Herzig, *Intermetallics* **8**, 1357 (2000).