

# Atomic Diffusion in B2-FeAl

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Diffusion processes in ordered intermetallic alloys are the object of sustained interest, particularly in view of a number of different mechanisms which have been proposed to describe the exchange of vacancies and atoms on the lattice. Methods like tracer [1] or NMR [2] measure diffusion on macroscopic scales and - in case of NMR - only in time. They are therefore not sensitive for the atomic jump mechanisms. Scattering methods like Mößbauer spectroscopy (MS) or quasielastic neutron scattering are much better suited to identify diffusion mechanisms. Due to their limited resolution, they are, however, only applicable for investigations at temperatures close to the melting point. Atomic scale x-ray photon correlation spectroscopy (aXPCS) is a microscopic, space resolved method that operates in the time- instead of the energy-regime [3]. It is therefore not subject to the limitations mentioned above.

Our goal was to use aXPCS to identify the dominant diffusion mechanism in B2-ordered FeAl. This material was object to long-standing investigations due to a unique combination of physical and mechanical properties, including high melting point, low density and good oxidation and corrosion resistance. It is therefore of great technological interest. In our group we investigated a number of iron-alumina phases [4, 5]. An Fe<sub>55</sub>Al<sub>45</sub> intermetallic alloy was studied by MS [5] at a homologous temperature of 0.85 (1363 K) which is a rather high fraction of the alloy's melting temperature  $T_m$ . In the recent experiment an Fe<sub>55</sub>Al<sub>45</sub> single crystal was measured in a vacuum furnace in transmission geometry. It was oriented with the  $\langle 111 \rangle$ -axis parallel to the incoming x-ray beam (see Fig. 1a). Due to the three-fold crystalline symmetry, measurements within  $60^\circ$  of the azimuthal angle are sufficient to obtain the full information about the autocorrelation time dependence. The distance sample-detector was 0.83 m. We used a Pixis-XB CCD camera with  $1340 \times 1300$  pixels,  $20 \times 20 \mu\text{m}^2$  pixel size and a read-out time of 2.3 seconds to collect the images. The exposure time was 3 s per frame. To avoid iron K-line fluorescence the beam energy was tuned to 7.05 keV. The sample was measured at 653 K which corresponds to only 0.42 of  $T_m$ .

A number of datasets was collected at the same scattering angle  $2\theta$  but for different azimuthal angles  $\phi$ , i.e. at different wavevectors  $\vec{q}$ . As we knew from our previous experiments [4, 5] and from ab initio simulations [6], iron diffusion in Fe-Al close to the stoichiometric composition is performed via jumps into a vacancy on the Al-sublattice. Actually one should expect in this case a sum of two exponential decays of the autocorrelation function (acf). It was, however, impossible to measure both components even with MS. This was due to the fact that the component with shorter decay time (this corresponds to a broad line in the energy domain of MS) is very weak. This effect was even more pronounced in the aXPCS measurement, as at only half of the homologous temperature the B2 intermetallic phase is still more perfectly ordered. Thus we expect to use a model containing only effective jumps of iron atoms on its own sublattice of the B2 phase.

The collected acfs were fitted with one exponential decay. Fig. 1b shows the angular dependence of the reciprocal correlation time  $\tau^{-1}$ . The lines in Fig. 1b are calculated using three different diffusion models: effective jumps over the elementary  $\langle 100 \rangle$  cube edge, effective jumps over the face diagonal  $\langle 110 \rangle$  and over the cube diagonal  $\langle 111 \rangle$ . As shown in Fig. 1b only the model of long cube-diagonal jumps fits the data and can therefore explain the acf's  $\vec{q}$ -dependence. The same holds for short jumps between NN-positions which are not shown in the figure. One should notice that in order to correctly interpret experimental aXPCS data a short-range order (SRO) of the sample must be known [3]. In the current evaluation we used a Monte Carlo technique to calculate SRO in

$\text{Fe}_{55}\text{Al}_{45}$  with interatomic pair-potentials derived from our previous studies [7]. The resulting SRO function is quite flat and did not change the model lines of Fig. 1b by more than 10%.

We conclude that due to the extremely high order of the  $\text{Fe}_{55}\text{Al}_{45}$  alloy and low homologous temperature of the sample, the contribution of farther effective jumps of iron atoms is significantly increased compared to the situation at much higher temperatures. Apparently this is due to the weak repulsing force between vacancies on the iron sublattice. This surprising result is in line with the results from our previous MS studies [5] where we could fit the data only assuming at least 20% of effective  $\langle 111 \rangle$  iron jumps in addition to the  $\langle 100 \rangle$  and  $\langle 110 \rangle$  jumps. Only at lower temperature solely available to an aXPCS measurement a very weak vacancy-vacancy interaction became apparently visible.

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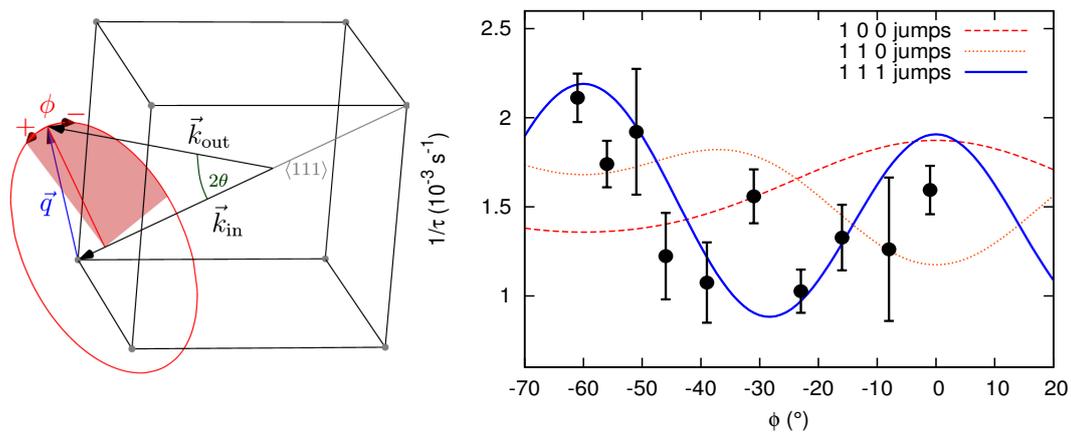


Figure 1: (a) Orientation of the sample relative to the incoming x-rays where the red shaded area marks the measured region and the solid red line corresponds to  $\phi = 0$ ; (b) reciprocal correlation times as a function of azimuthal angle  $\phi$  measured at 653 K together with different model lines.

## References

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