ESRF

	Experiment title: Atomic diffusion in B2-AuMg measured by XPCS	Experiment number: HS-4357
Beamline: ID10	**Date of experiment**: from: 16.11.2011 to: 22.11.2011	**Date of report**: 01.09.2016
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We proposed to study atomic diffusion in Au_xMg_{1-x} intermetallic alloys by atomic-scale X-ray photon correlation spectroscopy (aXPCS) in order to determine the diffusion mechanisms on both sides of the stoichiometric composition. Measurements on the prepared $Au_{64}Mg_{36}$ sample were not successful due to an overall low intensity and a very small speckles contrast β of the scattered X-rays. This was because the sample, which was prepared as thin as technically possible considering the softness of this single crystal, was a very strong absorber of 8 keV radiation. Instead, we measured during the beamtime HC-885 in April 2013 an equivalent B2-ordered phase $Ag_{58}Mg_{42}$. The speckles contrast β was significantly higher due to some improvements in the beamline setup.

The single crystal of $Ag_{58}Mg_{42}$ intermetallic alloy was oriented with its [110] direction normal to the surface. All measurements were done using the iKon-M CCD chip with a sample-to-detector distance of 67 cm. Exposure times were between 4 s for small angles and 8 s for angles larger than $2\theta = 8°$. The illuminated area on the sample was determined by slits of 20×20 μm^2. Measurements were taken at 423 K.

B2 alloys are usually considered either to be of the triple-defect type, where antisite atoms exist only on one sublattice and vacancies only on the other, or to be of the anti-structure type, where constitutional defects are formed as antisites for an excess A or B atoms, respectively [1]. Ag–

Mg alloys are usually assigned to the second class [2] but some authors report a hybrid behavior. The best fit was achieved mixing ⟨1 1 0⟩ and ⟨1 0 0⟩ effective jumps in the proportion 3:1. Our measurements suggest that chemical short-range order is rather weak in this system, thus we assumed that the SRO is constant $I_{SRO}(\mathbf{q}) = 1$. The resulting simultaneous fit to all data, i.e. to the azimuthal and to the polar scans is shown in Fig. 1.
As can be seen from Fig. 1, ⟨1 1 0⟩ jumps are dominant in $Ag_{58}Mg_{42}$ with and addition of ⟨1 0 0⟩ jumps. The diffusion coefficient at 423 K is $2.54(9)\times10^{-23}$ m^2s^{-1} [3].

Concluding, the microscopic diffusion mechanism in Ag–Mg is similar to that of Fe–Al alloy at high temperatures (above 1200 K) [4] but definitively different than in Fe–Al at about 700 K [5]. One can presume that similar atomistic mechanism is responsible for diffusion in Ag–Mg and in moderately ordered Fe–Al [4]. This mechanism takes place via correlated exchanges of a vacancy leading to farther effective jumps of the majority atoms. The precise ratio of frequencies of ⟨1 1 0⟩ to ⟨1 0 0⟩ jumps depends on the particular values of the exchange energy between both atomic species and a vacancy. This is definitely different than in Fe–Al [4], where ⟨1 1 0⟩:⟨1 0 0⟩ was 2:1 instead of 3:1 in an Ag–Mg intermetallic alloy.

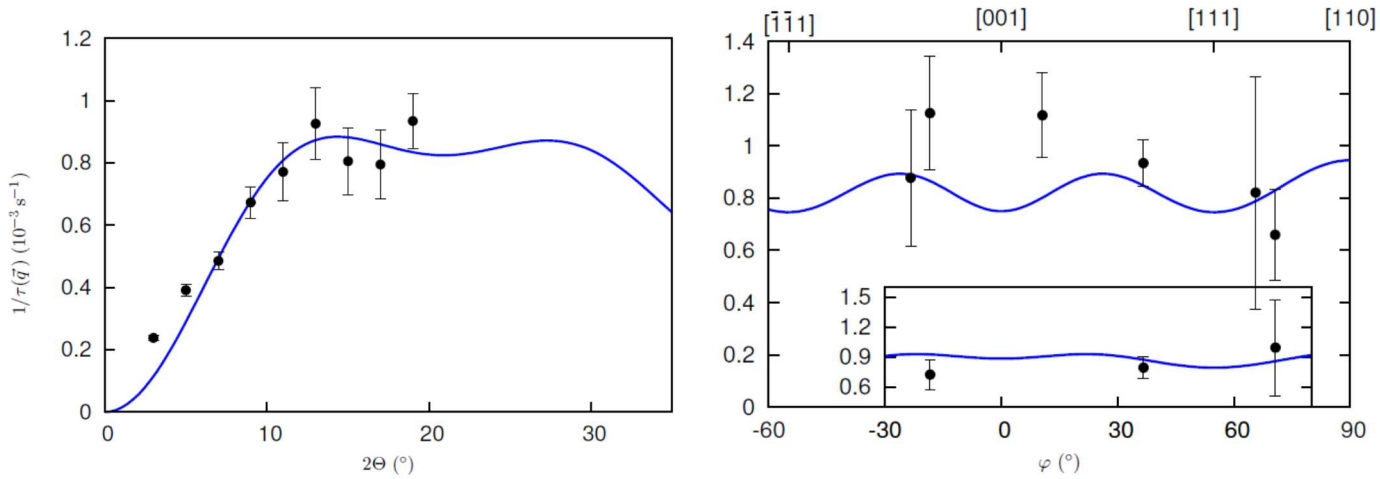

Fig. 1 (left) Inverse correlation time as a function of scattering angle 2θ; (right) as a function of azimuthal angle φ for 2θ = 19° and 2θ = 17° (insert). The simultaneous fit with an atomistic jump model described in the text is shown by the blue line. Figures taken from M. Stana PhD Thesis [3].

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References

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