ESRF	**Experiment title:** Studying diffusion by scattering of synchrotron radiation into Bragg directions	**Experiment number:** HS-869
Beamline: ID22	**Date of experiment:** from: 14/7/99 to: 20/7/99	**Date of report:** 20/8/99
Shifts: 14	**Local contact(s):** Helge Thiess, Tanja Asthalter	*Received at ESRF:* 3 0 AOUT 1999

Names and affiliations of applicants (* indicates experimentalists):

G. Vogl, Institut f. Materialphysik d. Uni Wien
*B. Sepiol, Institut f. Materialphysik d. Uni Wien
*M. Kaisermayr, Institut f. Materialphysik d. Uni Wien
*M. Sladecek, Institut f. Materialphysik d. Uni Wien
R. Rüffer, ESRF Grenoble

Report:

Nuclear Resonant Scattering of synchroton radiation (SR) is a valuable tool to determine atomic motion in solids [1]. Jump rates and jump vectors can be directly obtained from the model calculations for the coherency loss during scattering. The coherent state after excitation of the system by a very short SR pulse is destroyed by diffusion leading to faster decay of the re-emitted intensity. In crystalline solids coherent scattering can be measured in forward and in Bragg directions. The reported experiment was planed to be a feasibility test of the diffusionally accelerated intensity decay on a Fe_3Si single crystal in the case of Bragg scattering.

In HS-869 experiment we have measured intensity decay in reflection geometry. The potential goal of this geometry would be an access to samples which cannot be prepared as thin foils.

Fe_3Si single crystal cut with its (111)-direction normal to its surface was enclosed by a furnace mounted on a goniometer head. The rocking curve of the crystal shows high mosaicity. The time spectra of 14.4 keV resonant photons were measured in (222) and (444) Bragg reflections at three different temperatures T_1=550°C, T_2=570°C and T_3=600°C.

The crystal-radiation interaction is described by the dynamical theory of nuclear resonant scattering (DTNRS) [2]. The intensity decays in the time domain measured in the vicinity of Bragg reflections are strongly accelerated in comparison to an isolated nucleus and the acceleration is angle-dependent. The influence of diffusion is incorporated in the theory through the momentum-energy self-correlation function [3], mirroring all dynamical effects in the sample. Fig.1 shows the measured time spectra together with the numerical fits based on DTNRS. The diffusional acceleration of the decay with increasing temperature can be clearly seen. Jump frequencies in Table 1 are in good agreement with the results obtained from earlier measurements in forward direction [1].

(222) Bragg direction	0.1 MHz (550°C)	1.2 MHz (570°C)	7.8 MHz (600°C)
(444) Bragg direction	0.5 MHz (550°C)	2.1 MHz (570°C)	5.0 MHz (600°C)
forward direction [1]	0.9 MHz (554°C)	3.8 MHz (585°C)	6.7 MHz (612°C)

Tab.1 Jump frequencies obtained from the measurements in Bragg directions together with the values from forward scattering measurements.

1. In the (222)-direction the measured time spectrum can be fully understood with the help of DTNRS. Due to the mosaic spread of the sample an averaging over scattering angles in the vicinity of the Bragg reflection should be performed.
2. In the (444)-direction the validity of DTNRS is reduced and corrections for the high mosaicity of the crystal have to be applied. The higher order reflection leads to a deeper penetration of radiation into the crystal. The crystalline planes inside the sample which are less accurate aligned contribute to the coherent scattering. Consequently this case shall be better understood with the help of the "kinematical approximation" [4], so far not applied.

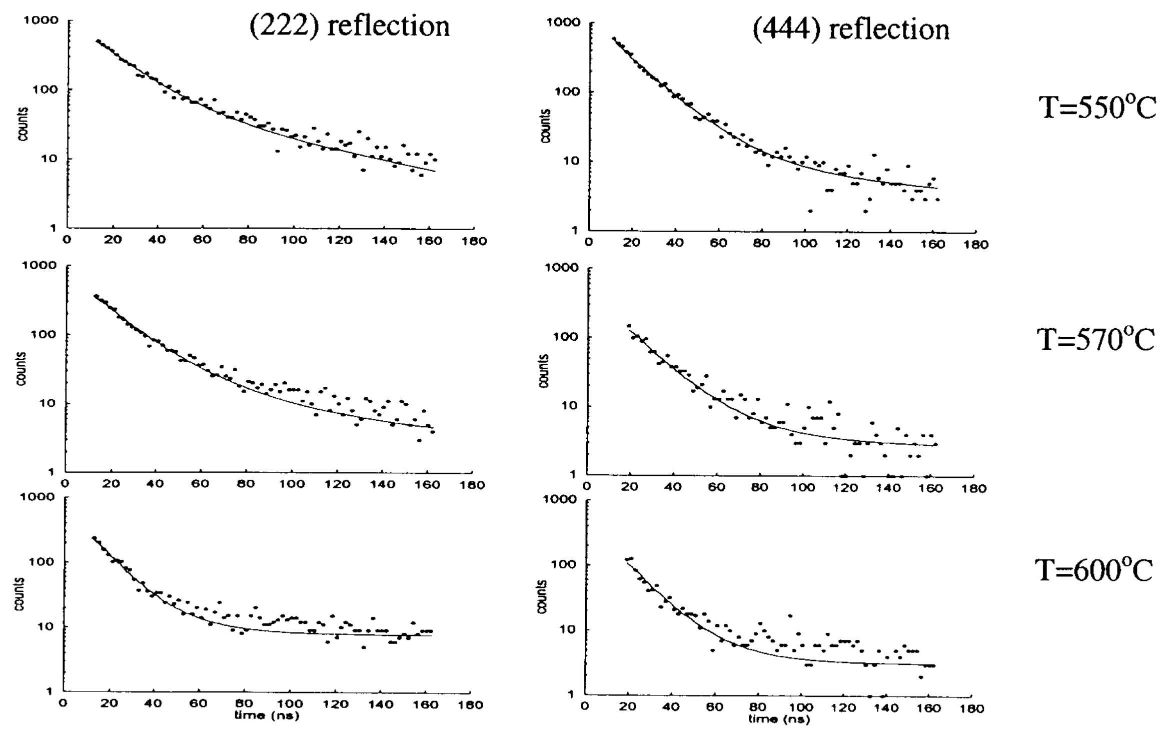

Fig.1 Time spectra of scattered synchrotron radiation into Bragg directions at three different temperatures

In conclusion we state that:

1. The diffusion mechanism can be investigated by measurements in Bragg directions.
2. The scattering mechanism can be understood with DTNRS. For higher-order reflections corrections due to mosaicity have to be applied.

[1] B.Sepiol, A.Mayer, G.Vogl, H.Franz, R.Rüffer, Phys.Rev.B, **57**, 10433 (1998)
[2] Y.Kagan, A.Afanas'ev, V.Kohn, J.Phys.C: Solid State Physics **12,** 615 (1979)
[3] V.Kohn, G. Smirnov, Phys. Rev. B **49**, 8768 (1994)
[4] Y.Kagan, A.Afanas'ev, I.Perstnev, Sov. Phys. JETP **27**, 819 (1968)