ESRF	**Experiment title:** Dynamics in Myoglobin studied by coherent inelastic scattering of synchrotron radiation with energy analysis by the Mössbauer effect	**Experiment number:** HS-272
Beamline: ID18	**Date of experiment:** from: 22.06.97 to: 26.06.97	**Date of report:** *06.08.97*
Shifts: 8	**Local contact(s):** Dr. R. Rüffer	*Received at ESRF:* 2 7 AOUT 1997

Names and affiliations of applicants (* indicates experimentalists):

*F. Parak, Fakultät f. Physik, E17, Technische Univ. München, D-85747 Garching
*U. van Bürck, Fakultät f. Physik, E15, Technische Univ. München, D-85747 Garching

Report:

Dynamics in Myoglobin studied by coherent inelastic scattering of synchrotron radiation with energy analysis by the Mössbauer effect

The Rayleigh scattering of synchrotron radiation is a coherent scattering method. The intermediate scattering function depends on the differences in the mean atomic positions $\vec{r}_j$:

$$I(\vec{k},t) = \sum_{j,j'} f_j f_{j'} \exp(i\vec{k}(\vec{r}_j - \vec{r}_{j'})) \exp(-k^2/2 < x_j^2 >) \exp(-k^2/2 < x_{j'}^2 >) \exp(k^2 < x_j(0) x_{j'}(t) >) \qquad (1)$$

f_j is the atomic scattering factor, $\vec{k}$ is the scattering vector and t the time. Typical distances $\vec{r}_j - \vec{r}_{j'}$ in a sample interfere by the first exponential to the maxima and minima in the scattering function. For myoglobin the first maximum is at $|\vec{k}| = 0.6\,\text{Å}^{-1}$, the second at $|\vec{k}| \approx 1.4\,\text{Å}^{-1}$. The scattered intensity also depends on the time dependent deviations $x_j(t)$ of the atoms from $\vec{r}_j$

A Fourier transformation of eq. 1 from time into energy space yields the dynamical scattering function. It depends on the energy of the excitations, of the correlations in x_j and, especially by the first exponential in eq.1, on $\vec{k}$. The inelastic Rayleigh scattering was used in a preceding experiment for the investigation of the temperature dependence of the phonon spectrum of myoglobin /l/. Up to now, these experiments had been performed at high scattering angles with momentum transfers between $|\vec{k}|$ = 2.9 $Å^{-1}$ and 14.3 $Å^{-1}$. Therefore the interpretation in this case was made within an incoherent approximation. At smaller angles correlations in the atomic distances and in the atomic motions are getting important.

In the present experiment again an amorphous sample of horse heart myoglobin hydrated to 0.4 g water / g protein was investigated. The scattered radiation was detected in an array of four APDs situated symmetrically around the direct beam. The covered scattering vectors $\vec{k}$ are given in Fig.1. Due to the very low counting rates of 0.3 s^{-1} in the maximum and a background of 0.06 s^{-1} only two angular regions could be studied in this beamtime. In both cases the statistics is not sufficient to yield information about correlations in the dynamical amplitudes.

References

/l/ K. Achterhold, C. Keppler, U. van Bürck, W. Potzel, P. Schindelmann, E.W. Knapp, B. Melchers, AI. Chumakov, A.Q.R. Baron, R. Rüffer, F. Parak, Eur. Biophy. J. Lett. 25 **(1996) 43-46**

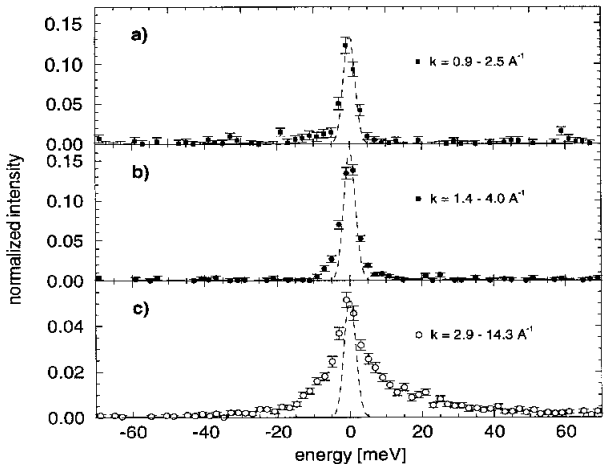

Fig.1: Phonon spectra at small and high scattering angles. The broken line represents the resolution function respectively.

a),b) Normalized spectra at small $\vec{k}$ with substracted background.

c) Normalized spectrum at high $\vec{k}$ showing incoherent scattering for comparison /1/. Notice the different intensity scales.