ESRF	**Experiment title:** Spectroscopy of synchrotron radiation scattered from KCN in its orientational disordered plastic phase with *neV* to μeV energy transfer	**Experiment number:** SC-320
Beamline: ID 18	**Date of Experiment:** from: 10/03/1997 to: 13/03/1997	**Date of Report:** 30/09/1997
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Report:

KCN is a simple molecular crystal with a pseudocubic sodium chloride structure at room temperature. It undergoes two phase transitions associated with the CN- electric dipole moment and the elastic quadrupole moment along the following temperature scheme: T = $300K$ pseudocubic, orientationally disordered (plastic) $\rightarrow T_{c1}$ = 168K electrically disordered (ferroelastic) $\rightarrow T_{c2}$ = *83K* electrically ordered (antiferroelectric). The rotational excitations of the CN-dumbbells overlap energetically with the ordinary "translational modes". Therefore, the rotational, librational and tunneling transitions cause an increased inelastic diffuse background in scattering experiments that diverges logarithmically when the upper phase transition is approached ([l] H. Jex et al. Solid State Commun. 36(1980)713; F. Wittmann and H. Jex Solid State Commun. 53(1984)407). At T_{c1} the elastic constant which is involved in the shear modes approaches zero $C_{44} \rightarrow 0$.
In our experiment at the nuclear beamline ID 18 we analysed the spectral distribution of that inelastic part in the *neV* to μeV- energy range by means of a nuclear resonant monochromator/absorber combination of two $FeBO_3$ crystals via the $14.4keV$ resonance line of ^{57}Fe. The first crystal - acting as a nuclear monochromator - was adjusted in the nuclear (333) Bragg reflection and the second one - used in transmission as a resonance absorber - was mounted in a high velocity transducer $(v_{max} = 1000\frac{mm}{s})$ for Doppler shifts up to $48\mu eV$. The synchrotron ran in the 16 bunch mode. We selected delayed photons from a time window between *9n.s* to 180ns into energy spectra. The nuclear hyperfine splitting and quantum beating of $FeBO_3$ is well known from the pioneering synchrotron work by ([2] U. v. Bürck et al. Phys. Rev. Letters 59(1987)355).
In our first experiment we measured the spectral resolution function of our two crystal monochromatar/absorber system at two Doppler velocities v_{max} = 400 (and $800)\frac{mm}{s}$ of a sinusoidal motion. Fig.1 presents the observed spectrum for the first velocity after folding of the collected data and after correction for the sinusoidal motion. We observe 4 lines with a maximum splitting of 42.5 (and 22) channels.

In the next experiments we adjusted the KCN crystal between monochromator and analyser in different Bragg scattering positions. We probed the (200), (400) and (600) reflections of KCN and found an effectively scattering domain with a halfwidth of 95arcsec and high scattering power in the (400) Bragg reflection. The crystal was mounted in a cryostat and temperature runs at T = 293K and 180K were taken with $400\frac{mm}{s}$ Doppler velocity and at T = *293K* and 170K with $800\frac{mm}{s}$ Doppler velocity. The data collected at *180K* with the Doppler velocity of $400\frac{mm}{s}$ are presented in Fig.2. We recognize the same 4 line structure after Bragg scattering from *KCN*. An unexpected feature of the spectra are the increased intensities in the wings of the four lines which are present in the gauge experiment and the KCN scattering as well. The spectral range outside the four lines from $\pm 400neV \Rightarrow dE \Rightarrow \pm 19.2\mu eV$ does not exhibit a significant peak structure. However, when the region around the four lines (inside the arrows of Fig.1 and 2) is integrated with the outer part as a reference (quasi background) line we find the following trend: in the gauge experiment the negative part below the reference dominates, while the positive contributions becomes increasingly dominant, when the phase transition at T_{c1} is approached. This holds for both Doppler velocities.
We conclude that the large Debye-Waller factor of KCN reduces the coherent elastic scattering, as temperature goes down! It may also indicate that the thermal diffuse inelastic scattering is concentrated in the sub-400neV energy range that could not be resolved in our experiment.
We thank the ESRF staff for their support and hospitality.

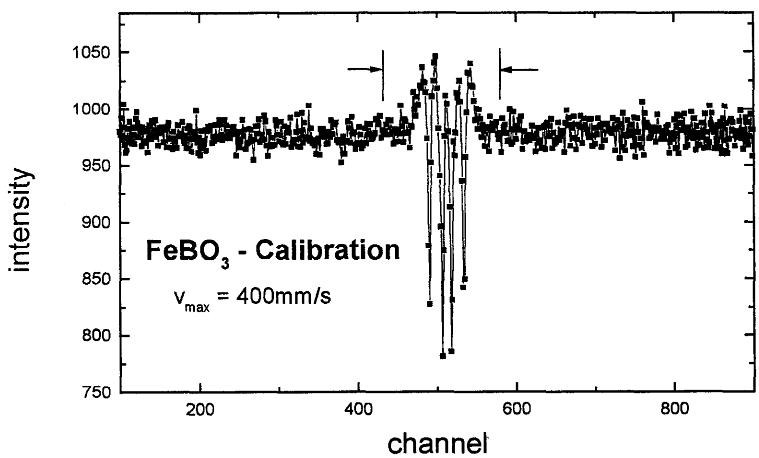

Fig.1:
Spectrum of $FeBO_3$ nuclear monochromatar/absorber system, normalized with the total number of counts $(1channel \hat{=} 18.75neV)$

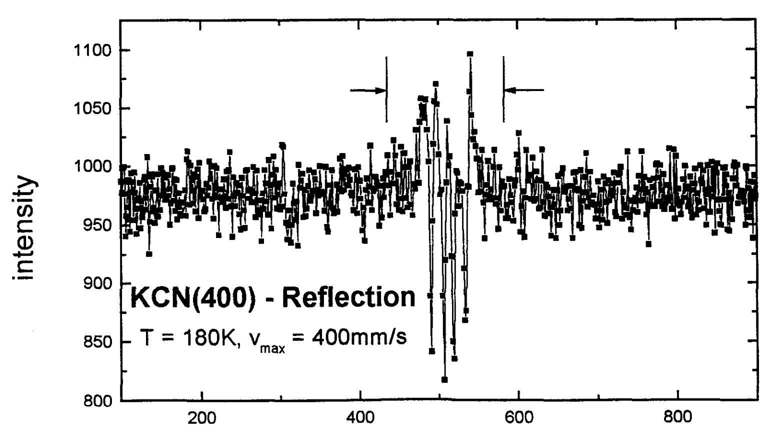

Fig.2:
Spectral intensity of KCN(400)-reflection, normalized with the total number of counts $(1channel \hat{=} 18.75neV)$