ESRF	**Experiment title:** Interplay of charge and magnetic ordering in $SmNiC_2$ and $NdNiC_2$	**Experiment number**: HC-4325
Beamline: ID28	**Date of experiment**: from: 07.04.2021 to: 12.04.2021	**Date of report**: 07.09.2021
Shifts: 18	**Local contact(s)**: Aleksandra Chumakova, Alexei Bosak (remote experiment)	*Received at ESRF:*

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Report:

In the current experiment we investigated the lattice dynamics in $SmNiC_2$ and $NdNiC_2$ by means of x-ray diffuse scattering (DS) and inelastic x-ray scattering (IXS). These two compounds – like many members of the RNiC$_2$ family, R=rare earth – display a strong interplay between charge density wave (CDW) ordering and magnetism [1]. More specifically, CDW order appears in $SmNiC_2$ ($NdNiC_2$) at 148 K (121 K) and is followed at T_c = 17.5 K (T_N = 17.2 K) by the ferromagnetic (antiferromagnetic) ordering of the rare earth moments [2,3]. In both cases, the CDW order is strongly influenced by the onset of the magnetic ordering. The goal of the experiment was to investigate the role of the phonons in driving the CDW transition and in mediating their interplay with the different types of magnetism.

The experiment was performed at the side and main station of the ID28 beamline, using a 17.79 keV incident x-ray beam. Single crystals of $SmNiC_2$ and $NdNiC_2$ grown by argon arc melting were used for the measurements. The samples were glued on a conically shaped glass rod and placed on a standard goniometer head mount. The DS and IXS measurements were performed in the temperature regime 80 K- 295 K. A liquid nitrogen cryostream was used for cooling the samples. The preliminary evaluation of the DS data was performed using the CrysAlis software.

We have started the experiment with a DS mapping of the reciprocal space of the two compounds. Selected results for $NdNiC_2$ are presented in Figure 1 which depicts the reconstructed maps of the (0.5 K L) reciprocal space plane. Intense DS signal is observed already at room temperature at q_1 = (0.5, 0.52, 0) and at q_2 = (0.5, 0.5, 0.5). Upon cooling the sample, the DS signal both at q_1 and at q_2 increases strongly. This comes in agreement with earlier x-ray diffraction investigations which have identified the formation of a superstructure related to the CDW ordering with propagation vector q, as well as weaker DS signal at q_2. Below CDW onset temperature T_{CDW} the DS signal at q_1 collapses into focused superstructure reflections. On the other hand, the DS signal at q_2, remains diffuse and does not evolve into satellite peaks upon further cooling. The DS data on $SmNiC_2$ revealed a very similar behaviour upon cooling.

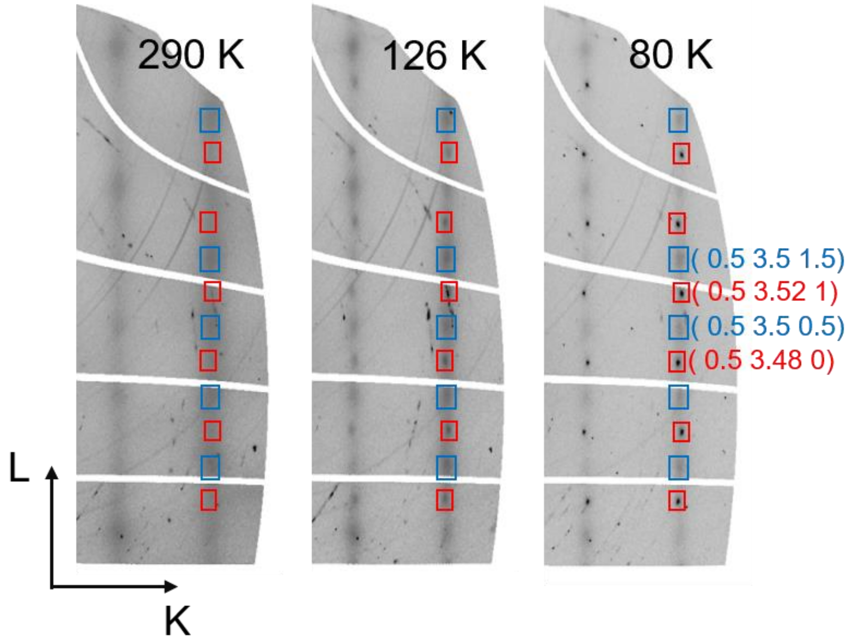

Figure 1: Reconstructed maps of the (0.5 K L) reciprocal space plane of $NdNiC_2$ at selected temperatures upon cooling. Red and blue boxes indicate the position of the DS signal corresponding to q_1 and q_2. The DS signal at q_1 evolves into sharp superstructure peaks of the CDW modualtion below T_{CDW}.

Having identified the regions of interest by temperature dependent DS, we have continued our investigation with energy-resolved IXS measurements on $SmNiC_2$ across the reciprocal space positions of the DS signal at q_1 and q_2 in the vicinity of the (0 4 0) Bragg peak. Selected IXS spectra along the [*x* 4-*x* 0] and [*x* 4-*x* *x*] cuts of the reciprocal space are given in Figure 2. A pronounced softening of a low energy acoustic phonon branch is observed around both q_1 and q_2. The temperature dependence of the IXS spectra indicates that the softening is complete at q_1 at the transition temperature. While the IXS measurements were done only on $SmNiC_2$, the similarity of the temperature dependent DS data on the two compounds suggest a comparable phonon behaviour also on $NdNiC_2$.

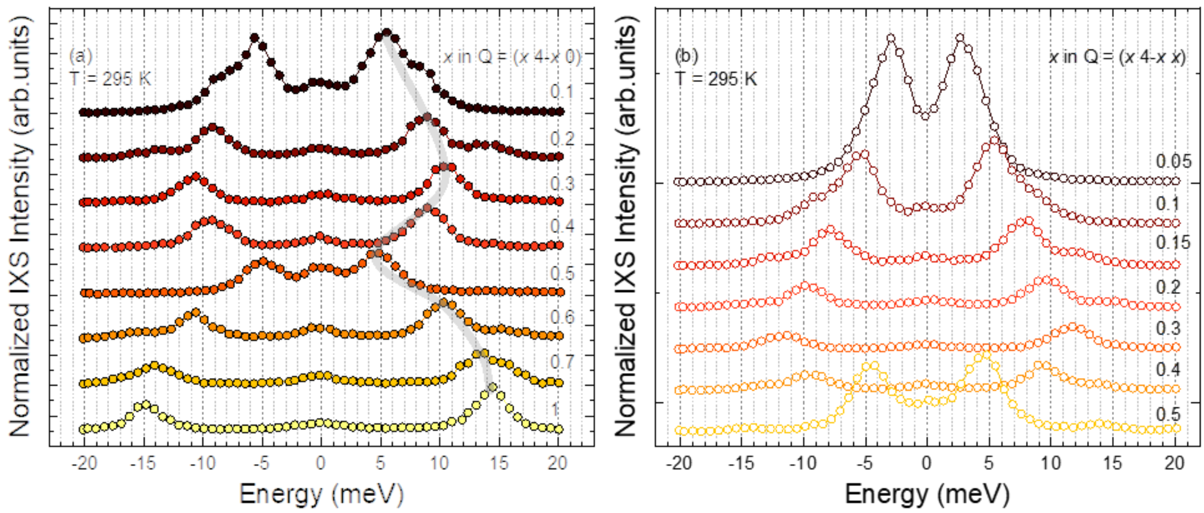

Figure 2: IXS spectra of $SmNiC_2$ recorded at 295 K from Γ = (0 4 0) along the (a) [1 -1 0] and (b) [1 -1 1] directions of the reciprocal space. The grey line in (a) is a guide-to-the-eye, highlighting the softening of the acoustic phonon close to q_1.

Unfortunately, during this remote experiment and the limited beamtime we did not have the time to explore the phonon behaviour below T_c/T_N. This is a very interesting issue, given that the CDW response to the magnetic ordering is different in the two systems. While in $SmNiC_2$ the CDW order is abruptly and completely destroyed below the onset of the ferromagnetic order, in $NdNiC_2$ it is gradually and only partially supressed by the antiferromagnetic order [2]. Future experiments will be required in order to clarify the phononic response in the magnetic states of the two compounds.

References:

[1] V. Babizhetskyy et al., Handbook on the Physics and Chemistry of Rare Earths, Vol. 52 (2017)

[2] S. Shimomura et al., PRL 102, 076404 (2009), N. Yamamoto et al., J. Phys. Soc. Jpn 82, 123701 (2013), A. Wolfel et al., PRB 82, 054120 (2010)

[3] Y. Onodera et al., J. Magn. Magn. Mater 182, 161-171 (1998)