



	<b>Experiment title: Lattice Dynamics of a High-Entropy Alloy</b>	<b>Experiment number:</b> HC-4327
<b>Beamline:</b> ID28	<b>Date of experiment:</b> from: 02/09/2020 to: 08/09/2020	<b>Date of report:</b>
<b>Shifts:</b> 18	<b>Local contact(s):</b> Alexei Bosak	<i>Received at ESRF:</i>
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## Report:

As stated in the proposal, the goal of this experiment was to complete our lattice dynamics study of the high-entropy alloy FeCoCrMnNi. Previous experiments using inelastic neutron scattering were limiting in the sense that all phonons were partly covered by a large incoherent scattering band, which persisted in multiple polarizations. Furthermore, initial scans made of longitudinal acoustic (LA) phonons showed a severe damping which was not present in transverse acoustic (TA) polarizations. Therefore, this ID28 experiment was meant to serve several purposes for us: (1) confirm that the textured band seen in the neutron experiments was indeed an effect of incoherent neutron scattering, (2) measure longitudinal phonons to investigate the damping, and (3) deduce intrinsic phonon lifetimes if possible, since the mosaic of our neutron sample did not allow for this under the instrumental resolutions used.

The single crystal sample was aligned into the [001][110] scattering plane in advance of the experiment. We remained on the [999] reflection for the duration of the experiment. The first few days were used to make an initial investigation at room temperature. We reconfirmed several phonons that had been measured previously by neutrons, and then focused on mapping four polarizations:

- LA phonons from the 002 Bragg peak, propagating along the [001] direction ( $LA_{001}$ )
- TA phonons from the 220 Bragg peak, propagating along the [001] direction, polarized along [110] ( $TA_{00\bar{1}}^{110}$ )
- LA phonons from the 220 Bragg peak, propagating along the [110] direction ( $LA_{110}$ )
- TA phonons from the 002 Bragg peak, propagating along the [110] direction, polarized along [001] ( $TA_{110}^{001}$ )

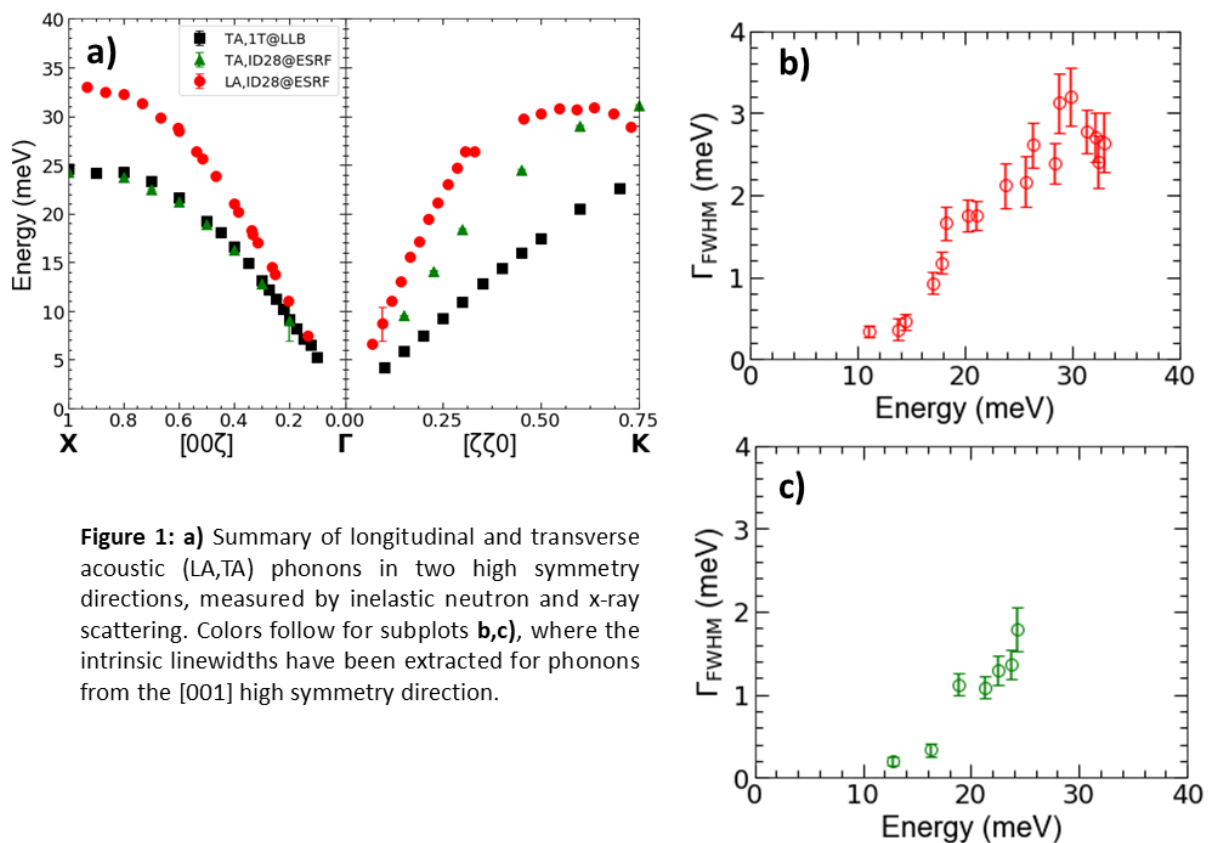
The remaining beamtime was spent on the temperature dependence of the  $LA_{001}$  and  $TA_{00\bar{1}}^{110}$  branches. Several phonons from each branch were measured at 100 and 15 K. Finally, during the last night, the analyzer resolutions were measured for our [999] configuration.

None of the scans taken during this experiment exhibited the large textured band seen in our neutron experiments, and therefore we concluded that this was indeed due to incoherent neutron scattering. Unlike in the neutron experiments, however, the LA phonons did not show the severe damping seen by the time-of-flight

neutron instrument. We have preliminarily concluded that this is an effect of having a sample with a poor mosaic that was “averaged” into the time-of-flight data.

As seen in Figure 1 **a)**, we now have a complete picture of the acoustic phonon dispersions in two high symmetry directions. No temperature dependence of these dispersions was found between 3-300 K, neither in the group velocities nor in the intrinsic widths. After fitting the data and accounting for instrumental, energy, and  $q$  resolution, intrinsic widths with temperature could be extracted (**b,c**), which turn out to be of the same order of magnitude as the binary alloy NiFe [1]. We are now writing an article summarizing all our neutron and x-ray results.

In parallel, we also measured the thermal diffuse scattering (TDS) of our samples from 90-500 K using ID28’s TDS side station. The results of this part of the experiment are still under investigation. However, preliminary findings point to evidence of Huang scattering surrounding the Bragg peaks.



**Figure 1:** **a)** Summary of longitudinal and transverse acoustic (LA,TA) phonons in two high symmetry directions, measured by inelastic neutron and x-ray scattering. Colors follow for subplots **b,c**), where the intrinsic linewidths have been extracted for phonons from the [001] high symmetry direction.

Reference:

[1] S. Mu *et al.*, Unfolding the complexity of phonon quasi-particle physics in disordered materials, npj Computational Materials **6**, 4 (2020).