EUROPEAN SYNCHROTRON RADIATION FACILITY

INSTALLATION EUROPEENNE DE RAYONNEMENT SYNCHROTRON

ESRF

Experiment Report Form

The double page inside this form is to be filled in by all users or groups of users who have had access to beam time for measurements at the ESRF.

Once completed, the report should be submitted electronically to the User Office via the User Portal: *https://wwws.esrf.fr/misapps/SMISWebClient/protected/welcome.do*

Deadlines for submission of Experimental Reports

Experimental reports must be submitted within the period of 3 months after the end of the experiment.

Experiment Report supporting a new proposal ("relevant report")

If you are submitting a proposal for a new project, or to continue a project for which you have previously been allocated beam time, you must submit a report on each of your previous measurement(s):

- even on those carried out close to the proposal submission deadline (it can be a *"preliminary report")*,
- even for experiments whose scientific area is different form the scientific area of the new proposal,
- carried out on CRG beamlines.

You must then register the report(s) as "relevant report(s)" in the new application form for beam time.

Deadlines for submitting a report supporting a new proposal

- 1st March Proposal Round - **5th March**
- 10th September Proposal Round - **13th September**

The Review Committees reserve the right to reject new proposals from groups who have not reported on the use of beam time allocated previously.

Reports on experiments relating to long term projects

Proposers awarded beam time for a long term project are required to submit an interim report at the end of each year, irrespective of the number of shifts of beam time they have used.

Published papers

All users must give proper credit to ESRF staff members and proper mention to ESRF facilities which were essential for the results described in any ensuing publication. Further, they are obliged to send to the Joint ESRF/ ILL library the complete reference and the abstract of all papers appearing in print, and resulting from the use of the ESRF.

Should you wish to make more general comments on the experiment, please note them on the User Evaluation Form, and send both the Report and the Evaluation Form to the User Office.

Instructions for preparing your Report

- fill in a separate form for each project or series of measurements.
- type your report in English.
- include the experiment number to which the report refers.
- make sure that the text, tables and figures fit into the space available.
- if your work is published or is in press, you may prefer to paste in the abstract, and add full reference details. If the abstract is in a language other than English, please include an English translation.

ESRF	**Experiment title:** Diffuse Scattering in NiCoMnTi all-d-Heusler alloys	**Experiment number**: MA5429
Beamline: ID15a	**Date of experiment**: from: 27.9.2022 to: 29.9.2022	**Date of report**:
Shifts: 3	**Local contact(s)**: Gavin Vaughan	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

David Koch* Technical University of Darmstadt - Material Science

Wolfgang Donner* Technical University of Darmstadt - Material Science

Report:

We conducted several single-crystal diffraction experiments for analyzing thermal diffuse scattering in $Ni_{37}Co_{13}Mn_{33}Ti_{17}$ single crystals. A x-ray energy of 60 keV was chosen. We measured two samples with different annealing conditions at different temperatures using the oxford cryostream. For each sample a single measurement was performed with rotating the sample with a constant speed of 1° per second around the phi axis with detector readout every 0,1°. Main experimental difficulties were to much intensity in the bragg reflections in terms of count rates an d saturation of the detector readout. Two enhance the overall intensity in the diffuse scattering data, therefore, we conducted at each temperature 16 single measurements, which were summed up in the data reconstruction afterwards. Applying the corresponding Laue symmetry to the data gives high quality reciprocal space maps of the diffuse scattering. In figure 1(a), the reciprocal space map at L=0 is shown, were the distinct features of the diffuse scattering are evident. The thermal diffuse scattering can be obtained with an high quality close to the bragg peaks, as indicated by the isosurface representation in figure 1(b). In contrast to other shape memory alloys, no maxima originating from a phonon soft mode are visible in the diffuse rods along [110] like directions. This does not change upon cooling. Additionally, the data shows, that the sample is in highly disorderd B2 structure, since no $L2_1$ short range order diffuse scattering is visible.

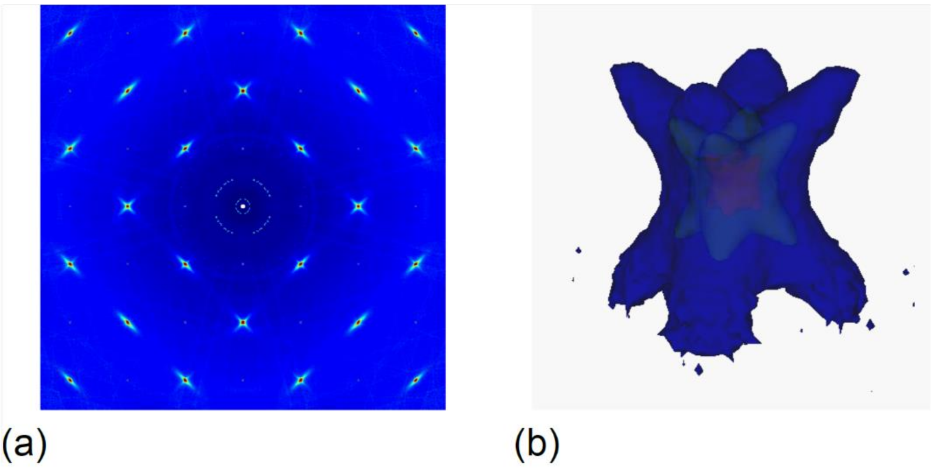

Figure 1:(a) Reciprocal space map at L=0 of $Ni_{37}Co_{13}Mn_{33}Ti_{17}$ at room temperature. (b) 3-dimensional view of the diffuse scattering of the (400) reflection.

By cooling below the phase transition temperature, the single crystal transforms to a monoclinic martensite, which results in a highly twinned sample. A exemplarly reciprocal space map is shown in figure 2. The satellites of the modulated martensite are along the [110] directions of the austenite, were the pronounced thermal diffuse scattering was found. After heating back to the high temperature phase, the single crystalline state is recoverd. The diffuse scattering data is used to analyse the elastic constants as precursors of the martensitic phase transition. Due to the high resolution and no artefacts from Bragg peaks the data is well suited. Unfortunately, the measurement series of the second sample was incomplete due to technical problems with the cryostreamer, nevertheless the dataset for the first sample is complete and from high quality.

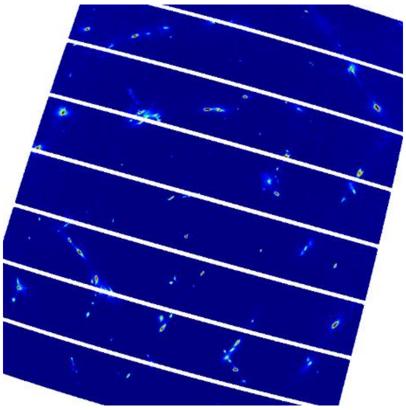

Figure 2:Reciprocal space map at 170 K of the twinned martensite.