ESRF	**Experiment title:** **Measurement of phonon dispersion in Ti-24Nb-4Zr-8Sn by inelastic X-ray scattering**	**Experiment number**: HS-4808
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Background

The phonon dispersion of pure β phase titanium at 1020°C has been measured [1], as has that of NiTi-based shape memory materials [2], and these measurements continue to support advances in understanding of elastic constants and transformation behaviour [3]. Despite widespread interest in alloys based on the titanium-group V/VI bcc system for the development of low-elastic modulus biomedical alloys [4], the phonon dispersion of a representative alloy at room temperature has never been measured. Doing so is expected to provide significant insight into control of elastic properties, as well as deeper understanding of martensitic transformations in titanium. Ti-24Nb-4Zr-8Sn (wt%) is an excellent case study for this purpose because it has the lowest polycrystalline Young's modulus yet measured in β phase titanium.

This inelastic X-ray scattering work is being carried out following previous synchrotron X-ray powder diffraction work [5] and is part of a project carried out by ANSTO and IMR, Shenyang, China, to research elastic properties of Ti-24Nb-4Zr-8Sn, especially non-linear behaviour in single crystals [6] at low stress.

Experimental overview

Several branches of dispersion curves in the bcc β phase of Ti-24Nb-4Zr-8Sn were acquired at 100K, 298K and 423K. For the 298K measurements, samples of two different oxygen content were measured. In all cases LA[111] and then TA1[112] and TA1[110] branches were measured for their relevance to, respectively, the β-ω and β-α″ transformations. Thereafter sufficient other branches were measured to define elastic constants of the β phase. The scope of measurements is shown in Table 1.

Treatment of Data

FIT28 was used to fit the raw data and define excitation energies, among other parameters. Use of the Damped Harmonic Oscillator function was necessary to account for the large damping that caused wide and flat peaks in many branches, especially those with low energy. In some cases a second excitation peak was also required to improve quality of fitting. The appearance of the dispersion curves is qualitatively similar to that of pure titanium at high temperature [1], with low energy TA1[110] and TA1[112] branches under 10 meV, and the pronounced anomaly in LA[111] where energy transfer falls to zero energy at q=2/3. An example of raw data and peaks fit in FIT28 are shown in Figure 1.

Dispersion curve sets are being prepared for publication, with additional first-principles modelling planned to provide explanation for the different nature of the soft modes and other anomalies as a function of oxygen concentration and temperature, and link these to the elastic properties.

Table 1: Number of data points measured for phonon branches

Planes	Mode	0.10w% O 100 K	0.10w% O 298 K	0.10w%O 423 K	0.18w%O 298 K
112	L		2		
112	T1	11	19	10	10
110	L	3	3	4	5
110	T1		5	7	5
001	L	3	9	7	3
001	T	3	10	7	5
111	L	11	23	14	11
111	T		10	3	3

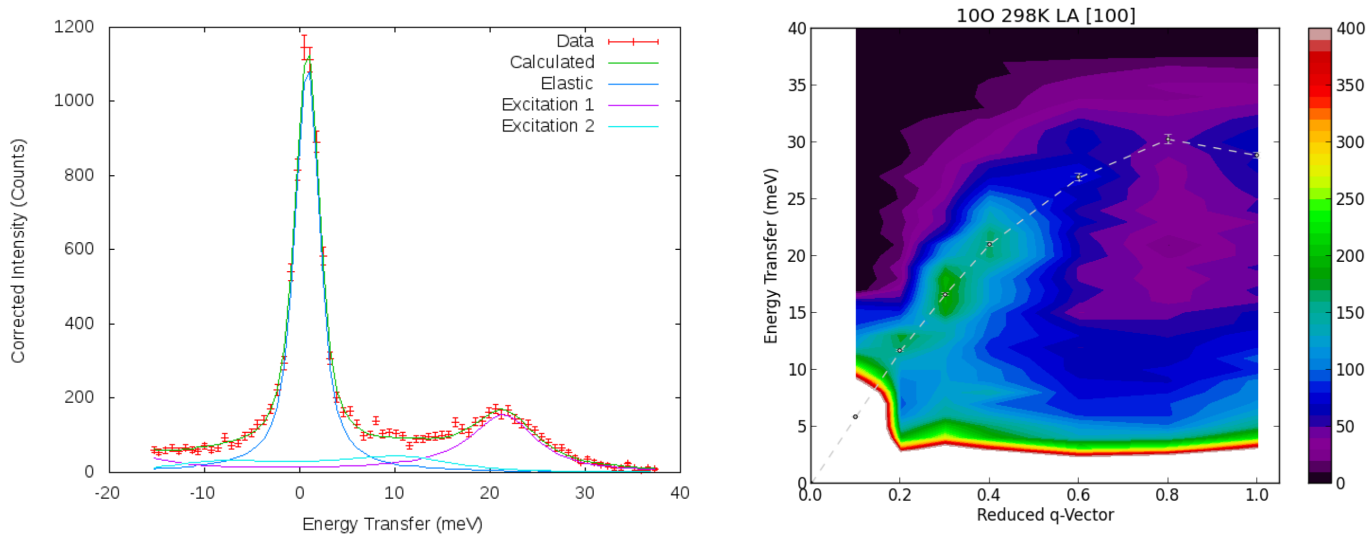

Figure 1: Inelastic scattering data from 0.10 wt%O, 298K, LA[100]: (left) FIT28 curve fitting at q=0.4; (right) contour plot of corrected intensity for all measurements along LA[100] branch.

References

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