Experimental report

17/02/2020

Proposal: **7-01-493**

Council: 10/2018

Title: Phonon dynamics in High Entropy Alloys

Research area: Physics

This proposal is a new proposal

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Samples: $Fe_{20}Cr_{20}Co_{20}Mn_{20}Ni_{20}$

Instrument	Requested days	Allocated days	From	To
IN6-SHARP	4	1	01/07/2019	02/07/2019

Abstract:

High Entropy Alloys (HEA), single-phase random solid solutions, characterized by excellent mechanical and magnetic properties, have revolutionized material science, and at the same time arisen new fundamental questions on alloy formation and the microscopic origin of such properties.

At this day no investigation exists of the lattice dynamics of an HEA, which can be thought of as the prototype of chemical disorder. Here we propose to measure the density of states of the HEA $Fe_{20}Cr_{20}Co_{20}Mn_{20}Ni_{20}$. Being intermediate between crystal and glass, presenting nanoscale elastic heterogeneities, like in a glass, but long range periodicity like in a crystal, the question whether there is a Boson Peak will be specifically addressed. This proposal is part of the PhD thesis work of S. Turner.

Generalized Vibrational Density of States of a High-Entropy Alloy

As stated in the original proposal, the goal of this experiment was to measure the generalized vibrational density of states (GVDOS) of our equimolar high-entropy alloy (HEA) FeCoCrMnNi as one part of our larger goal to study the lattice dynamics of high-entropy alloys. With the two days that we were assigned, we measured a powder sample of FeCoCrMnNi (a = 3.6 Å, space group 225) at 300 K, 200 K, and 100 K using an incoming wavelength of λ = 5.1 Å. We then took empty can measurements at all three temperatures. (As seen in the graphs below, we ran out of time for good statistics at 100 K.)

Fig. 1 depicts the GVDOS of our sample as described above. The Mantid environment for IN6 was used, and the scripts included both empty can subtraction and an initialization using a recent vanadium measurement. For all three temperatures we find two broad peaks at 20 and 30 meV. We believe these are related to optical branches of the material, as these match the peaks seen in our phonon dispersion energy scans measured on 1T@LLB. Perhaps the most striking feature of **Fig. 1**, however, is the fact that there is no ω^2 dependence at low energy. Not only is there no ω^2 dependence, but the slope of the almost-linear dependence seems to increase with decreasing temperature.

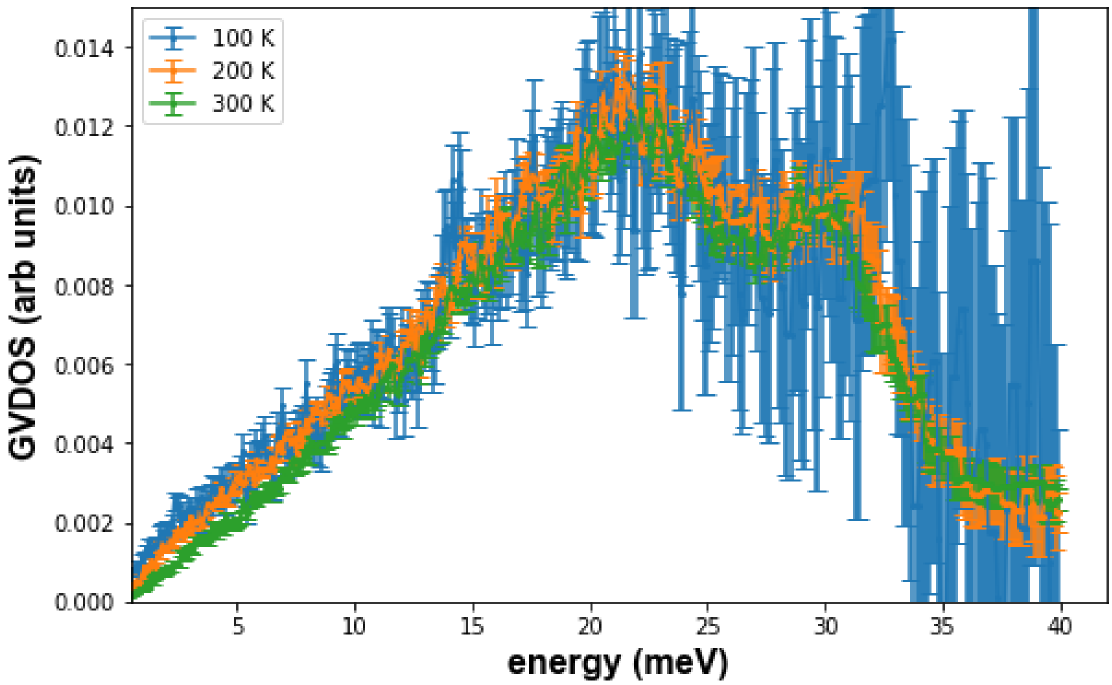

Fig. 1: GVDOS measurements (λ = 5.1 Å) taken at 300 K (green), 200 K (orange), and 100 K (blue). GVDOS calculation was made by using the Mantid environment for IN6 with an empty can subtraction.

This peculiar behavior, however, does not appear to be a trend in HEAs, as the GVDOS of the very similar HEA FeCoCrNi (the same but without Mn) was measured by Lucas *et al.* (M.S. Lucas *et al.,* Journal of Applied Physics 109, 07E307 (2011)). As seen in **Fig. 2**, the HEA FeCoCrNi does exhibit an ω^2 dependence at low energy, and then follows the same trend as our measurement starting from 20 meV. Besides the one missing element, Mn, the measurement by Lucas *et al.* was also not done by neutron scattering but by Nuclear Resonant Inelastic X-ray Scattering (NRIXS). This leads us to preliminarily conclude that the excess of signal that we see between 0-20 meV that causes the near-linear dependence is actually magnetic signal that we have picked up with neutrons. This is supported by the fact that the signal increases with decreasing temperature.

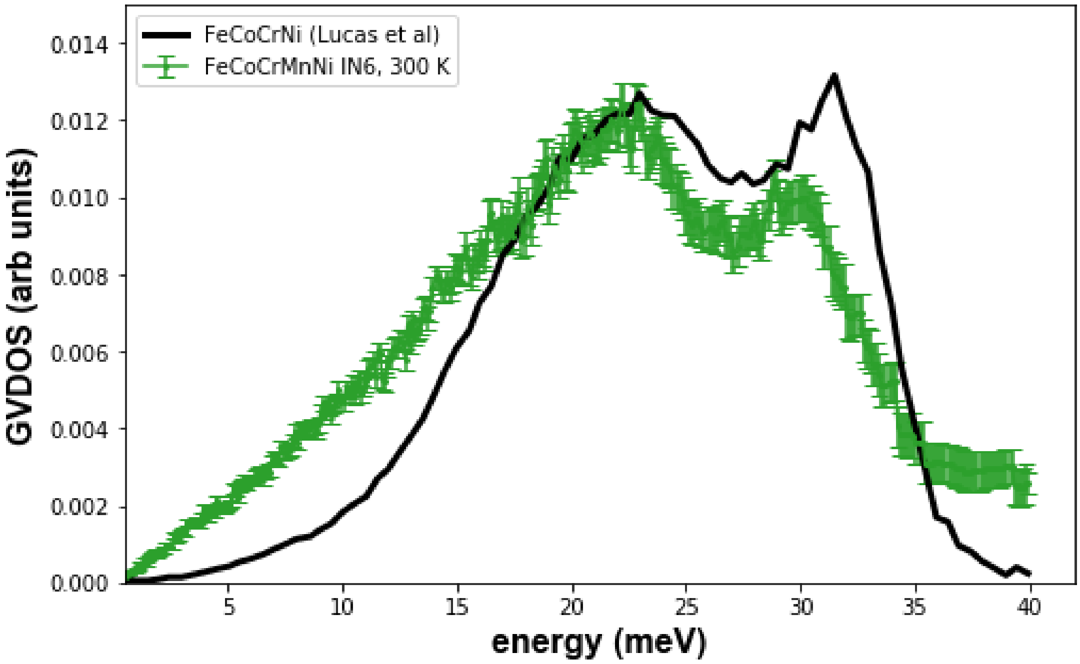

Fig. 2. Comparison of our FeCoCrMnNi GVDOS measurement on IN6 (green) to one made for the similar high-entropy alloy FeCoCrNi (black) by Lucas *et al.* (M.S. Lucas *et al.,* Journal of Applied Physics 109, 07E307 (2011)).

The analysis of this IN6 measurement will continue during the course of S. Turner's thesis, as it appears that a large component of the signal we have measured is due to magnetic effects of the material.

Note: To follow the progression of this project, see the experiment report for #7-01-505.