used to calculate the moduli values as a function of compostion based on the Voigt-Reuss-Hill approach.

2.3 Experimental

2.3.1 Ti-Nb sample preparation

To study the effect of the metastable phase formation, two sets of Ti-Nb alloy samples at 0.1, 0.12, 0.18, and 0.2 mole fraction of Nb using pieces of Ti (99.8 % Ti Alfa Aesar, Stock No. 00241 for set one, and 99.8 % Sigma Aldrich, Stock No. 305812 HELP) and Nb (99.8 % Sigma Aldrich, HELP, for set one and set two). Two different titanium pieces were used because the Alfa Aesar titnaium pieces were out of stock but they both had the same purity and thus should not lead to any issues with the data analysis. The alloyed samples were arc melted (MAM1, Edmund Buhler GmbH, Germany) under argon atmosphere. The alloys were machined into a cylindrical shape (0.7 inches in diameter and 0.7 inches in thickenss). The samples were then heat treated using a Lindberg 59544 tube furance. The tube was made of Al_2O_3 and was under vaccuum. The samples were annealed at 1273 °K for 24 hours. The samples from set 1 were quenched in water to form the α" phase. The samples in set 2 were slow cooled to form the ω phase.

2.3.2 Neutron Scattering

2.3.2.1 ARCS

The inelastic neutron scattering measurements were carried out using the Wide Angular-Range Chopper Spectrometer (ARCS) at the Spallation Neutron Source (SNS) at Oak Ridge National Laboratory. ARCS is a time-of-flight spectrometer meaning that the neutron beam and energy are fixed and the ARCS detectors measure the neutrons final position and the time elapse. From this information, the data output on ARCS is a plot of the momentum and energy of the neutrons. The measurements were taken with the samples loaded in a customized vanadium sample holder. The holder was mounted into the furnace and kept under vacuum throughout all measurements. Two incident neutron energies, $E_i = 25meV$ and $E_i = 50meV$, were used at each temperature (300, 500, 700, 900, 1110 K). Vanadium was chosen

for the sample holders because vanadium has a very low coherent scattering for neutrons. The empty vanadium sample holder was measured at the same conditions at each temperature. The measurements of the scattering from the empty sample holder and a linear background from the ARCS instrument were subtracted from the data of the sample.

2.3.2.2 Data Analysis

From the corrected momentum and energy plots of the samples, the diffraction patterns and phonon density of states were obtained.

Diffraction is prominently an elastic scattering process. So the intensities of neutrons, with no change in energy, at each momenta are calculated and modeled as a Gaussian function [84, 85]. In the present work, each alloy sample contained some combination of the bcc, hcp, α" and ω phases. In order to obtain the phase fractions, diffraction patterns, from the literature, of Ti and Nb in each of the individual phases were combined and fit to the diffraction pattern of the alloy in question. In order to do the fitting, the distance between scattering planes was taken into account for each phase. By fitting the literature diffraction patterns to the diffraction pattern of the alloys being studied the phase fractions were obtained.

From the energy vs momentum plots the phonon DOS of states was obtained using an iterative method to remove the elastic and multi-phonon contributions to the phonon DOS and thus plot just the one-phonon DOS [86, 87]. First, a trial phonon DOS from the momenta vs energy plots was used to calculate the time dependent self-correlation function ($G(t)$) and the mean square atomic displacement $\langle u^2 \rangle$. The trial single-phonon DOS (S'(ϱ)) was obtained by modifying the measured signal (S(ϱ)) by suppressing the elastic peak and contraining S(ϱ) such that dS(ρ)/dρ=0 when $\varrho \to 0$ according to the hydrodynamic limit. Using the trial phonon DOS, $G(t)$ was expressed by [88, 89]:

$$G(t) = \int_{-\infty}^{\infty} d\varrho \frac{Z(\varrho)}{\varrho} n(\varrho) e^{-i\varrho t} \tag{2.39}$$

where $Z(\varrho)$ is the phonon density of states as a function of phonon frequency ϱ and $n(\varrho)$ is the thermal occupancy factor. From $G(t)$ the dynamic structure factor from the incoherent scattering was calculated by [88, 89]:

$$\overline{S}^{inc}_{total}(\varrho) = \sum_{\theta} \frac{1}{2\pi\hbar} e^{-Q^2(\theta,\varrho)\langle u^2\rangle} \int_{-\infty}^{\infty} dt e^{-i\varrho t} e^{\hbar^2 Q^2(\theta,\varrho) G(t)/2M} \left[e^{\frac{-t^2}{2}\left(\frac{\triangle E(\varrho)}{2\hbar}\right)^2} \right] \quad (2.40)$$

where $e^{-Q^2(\theta,\varrho)\langle u^2\rangle}$ is the Debye-Waller factor described the mean square atomic displacement [87]. The anisotropy in the Debye-Waller factor was neglected because the resulting errors were negligible [88]. M is the mass of a neutron, $\hbar$ is Planck's constant and the bracketed area is the Gaussian instrument energy resolution. Q is defined by [88, 89]:

$$Q(\theta, \varrho) = \sqrt{\frac{2M}{\hbar^2}\left(2E - \hbar\varrho - 2E\sqrt{1 - \frac{\hbar\varrho}{E}} cos(2\theta)\right)} \quad (2.41)$$

From $G(t)$, the incoherent one-phonon $\overline{S}^{inc}_1$ and elastic scattering $\overline{S}^{inc}_0$ were determined. $\overline{S}^{inc}_0$ and $\overline{S}^{inc}_1$ are the zeroth and first order terms in the Taylor expansion of the $\overline{S}^{inc}_{total}$ when $G(t) = 0$ and the multi-phonon incoherent scattering (S^{inc}_m)contribution can be calculated by [88, 89]:

$$\overline{S}^{inc}_m = \overline{S}^{inc}_{total} - \overline{S}^{inc}_0 - \overline{S}^{inc}_1 \quad (2.42)$$

The calculated $\overline{S}^{inc}_m$ is then a good approximation for the multiphonon coherent scattering contribution and the single phonon DOS was calculated by:

$$Z(\varrho) = S_1(\varrho) * \frac{\varrho}{n(\varrho)} \quad (2.43)$$

The procedure was repeated three times to converge the phonon DOS based on previous recommendations that showed three iterations were enough to converge within statistical errors [88, 89].