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's original position 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 length for neutrons and would not interact with the samples at the high temperatures being measured. The empty vanadium sample holder was measured at the same conditions at each temperature. The output of momentum and energy of the neutrons was corrected for the empty can scattering as well as the ARCS background.

2.3.2.2 Data Analysis

From the corrected momentum and energy plots of the samples, the diffraction patterns and phonon density of states can be 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 Guassian 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 are combined and fit to the diffraction pattern of the alloy in question. In order to do the fitting, the distance between scattering planes is taken into account for each phase. By fitting the literature diffraction patternsto the diffraction pattern of the alloy being studied the phase fractions are obtained.

From the energy vs momentum plots the phonon DOS of states can be obtained in a few different ways. In the present work an iterative method is used to remove the elastic and multi-phonon contributions to the phonon DOS and thus plot just the one-phonon DOS [86, 87]. In order to obtain the one-phonon DOS, an iterative process was done that approximates the multi-phonon contribution and subtracts that and the elastic contribution from the total scattering to obtain the single-phonon DOS. 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 $\langle u^2 \rangle$. $G(t)$ 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 $e^{-Q^2(\theta,\rho)} \langle u^2 \rangle$ 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 bracked area has the $\triangle E$ which is the Gaussian instrument energy resolution of variable width. 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 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 as well. The elastic contribution was then total dynamical structure factor was scaled to match the incoherent dynamical structure factor and the elastic contribution was subtracted. From there the multiphonon contribution was subtacted leaving the new one-phonon DOS. This new one-phonon DOS was used to recalculate the multiphonon contribution. 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].