Resonance Raman Spectroscopy of 3D and 2D Niobium Diselenide

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Niobium diselenide ($NbSe_2$) is a metallic transition metal dichalcogenide with a charge density wave state below 33.5 K [1] and a superconducting state below 7.2 K in bulk [2]. In this work, we examine the excitation wavelength dependence of the Raman modes of $NbSe_2$. In $NbSe_2$ the three principal Raman modes are the A_{1g}, an out of plane vibration of the selenium atoms, E_{2g}, an in plane vibration of the niobium and selenium atoms, and the soft mode, a two-phonon second order scattering process. We investigate the intensity, Raman shift, and FWHM of these three Raman modes as a function of polarization and excitation energy from 1.6 eV to 2.7 eV. We find that the A_{1g} mode has a peak intensity when excited by longer wavelengths in the visible range. Conversely, the E_{2g} mode has a peak intensity when excited by shorter wavelengths in the visible range. A change in the relative intensity of the A_{1g} and E_{2g} vibrational modes with excitation wavelength has been observed previously in semiconducting molybdenum disulphide (MoS_2) [3]. As in this previous work on MoS_2, we relate the symmetries of the vibrational modes with the band structure using reflectance contrast spectroscopy. We find surprising similarities between the band structure of $NbSe_2$ and MoS_2. Finally, we present the thickness dependence of the reflectance contrast and Raman spectra of $NbSe_2$. Understanding the symmetries of Raman modes and the band structure is especially important for $NbSe_2$ which undergoes major band structure changes when transitioning to the charge density wave phase and superconducting phase.

References

[1] Wilson, J. A., Di Salvo, F. J., Mahajan, S., *Adv. Phys.*, 32 (1974) 882
[2] Soto, F., *et al.*, *Physica C*, 460 (2007) 789
[3] Carvalho, B. R., Malard, L. M., Alves, J. M., Fantini, C., Pimenta, M. A., Journal, Issue (Year) page

Figures

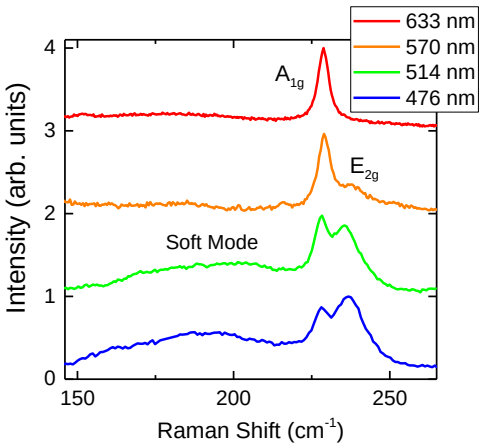

Figure 1: Raman spectra of bulk $NbSe_2$ for four different excitation wavelengths. The Raman spectra have been normalized to the highest value in range and vertically offset for clarity.

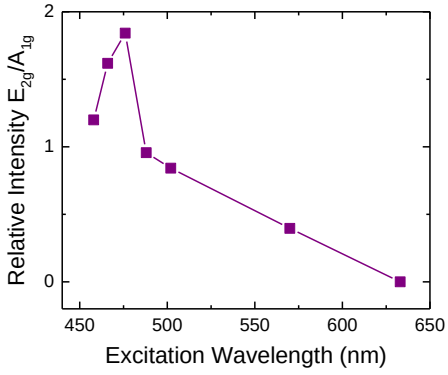

Figure 2: Relative intensity of the E_{2g} and A_{1g} Raman modes of bulk $NbSe_2$ as a function of wavelength.