

# Materials Science & Engineering Thesis Defense

## Ultrafast Xray Diffraction Study of Charge Density wave in TiSe<sub>2</sub> by Observing Electron-Phonon Coupling


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### Abstract

Transition Metal Dichalcogenide TiSe<sub>2</sub> can exhibit periodic lattice distortion also known as Peierls distortion which gives rise to charge density wave (CDW) superlattice formation. The origin of the CDW order in TiSe<sub>2</sub> is whether due to traditional Fermi surface nesting or excitonic insulator formation or indirect Jahn Teller effect, or electron-electron and electron-phonon interactions is a debatable issue. In TiSe<sub>2</sub> however it has been confirmed the formation of a condensate of electron-hole pairs with nonzero total momentum, in which the Peierls distortion, electron-electron interactions, and lattice pinning effects playing key roles. The main objective of this work is to understand the fluctuations due to electron-phonon interactions from the phonon dispersion and from thereon we look to forward in finding an answer for CDW origin. These fluctuations (or, oscillations) are manifested in the optical reflectivity, conduction band energy and Bragg diffraction. We have observed fluctuations (and couplings) by exciting the TiSe<sub>2</sub> lattice with laser by exciting the carriers and perturbing the electronic structure and used X-ray for probing the fluctuations and knowing how laser pulse control these fluctuations. We used ultrashort laser pulse having the femtosecond pulse duration and high average brightness of LCLS, SLAC to change the equilibrium CDW amplitude to a new equilibrium position (the DECP mechanism) followed by hard X-rays of LCLS to probe the momentum-resolved diffuse scattering, modeled as a momentum-dependent phonon population. In our experiment femtosecond technique Time resolved X-ray diffuse scattering has been employed for probing the mean-square fluctuations as a function of wavevector in diffuse scattering near the transition temperature for understanding electron – phonon coupling, how phonon dispersion looks near the region of Kohn Anomaly and other associated anisotropic electron-phonon interactions.



October 26, 2021; 1:15 PM; ERC 593