Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Mapping the Fermi Surface in Nb by Tracking Kohn Anomalies with Neutron Scattering[1] IYAD AL-QASIR, OLIVIER DELAIRE, VICKIE LYNCH, DOUGLAS ABERNATHY, MATT STONE, Oak Ridge National Laboratory — Electron-phonon interaction in metals is a subject of interest for theoretical and experimental investigations. Phonons in Nb show Kohn anomalies due to the electron-phonon interaction. In this work, we are tracking Kohn anomalies in Nb in the full Brillouin zone experimentally and computationally and relating it to the Fermi surface. We measured the 4-dimensional scattering function, $S(\vec{Q},\omega)$ of Nb as a function of temperature, using time of flight inelastic neutron scattering. The 4D data allow us to map phonon dispersion relations along any direction in the full Brillouin zone. In parallel, density functional theory was used to calculate the electronic band structure and Fermi surface, as well as the phonon dispersion relations and line-widths. We present a quantitative comparison, taking into account experimental resolution. These results point to a new avenue of mapping the Fermi surface and electron-phonon coupling in bulk crystals, complementing existing techniques.

[1]Funding from the US DOE, Office of Basic Energy Sciences, Materials Science and Engineering Division

Iyad Al-Qasir
Oak Ridge National Laboratory

Date submitted: 18 Nov 2012 Electronic form version 1.4