

Abstract Submitted
for the 4CF15 Meeting of
The American Physical Society

Optical Constants and Band Structure of NiO AYANA GHOSH, CAYLA NELSON, LINA ABDALLAH, STEFAN ZOLLNER, New Mexico State University — Using spectroscopic ellipsometry and transmission measurements, the optical constants (absorption coefficient, complex refractive index, dielectric function) of bulk NiO from 0.08 to 6.5 eV are determined. To obtain an accurate dielectric function of NiO, elastic scattering by oxygen bubbles was ruled out by analyzing the data. The effects of surface roughness were also removed to calculate the same. A direct band gap of 0.85 eV was found from transmission and assigned to direct interband transitions from the Ni-O hybrid valence band states to the Ni 4s conduction band at the center of the Brillouin zone. At 4 eV, we find the well-known charge transfer gap from the lower to the upper Hubbard band. Several intermediate sharp peaks were also found. The temperature dependence of the NiO charge transfer gap is similar to the E1 gap of Si between 100 and 700 K. At higher temperatures, heating NiO in vacuum leads to sublimation, which has drastic irreversible consequences for the pseudodielectric function of the sample, including a strong Ni nanoparticle plasmon peak at 2 eV.

Ayana Ghosh
New Mexico State University

Date submitted: 09 Sep 2015

Electronic form version 1.4