Abstract Submitted
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Dielectric function of NiO and Si from 25 meV to 6 eV: What's the difference?[1] S. ZOLLNER, C.M. NELSON, T.I. WILLETT-GIES, L.S. ABDALLAH, New Mexico State University, A. GHOSH, University of Michigan-Flint — Using spectroscopic ellipsometry, we determined the dielectric function of bulk NiO and Si from 25 meV to 6 eV to compare their lattice dynamics and electronic structure. From 0.7 to 6.6 eV, we studied the temperature dependence of the dielectric function from 77 to 800 K. In the visible and UV spectral region, both materials have a remarkably similar dielectric function: Both materials are transparent in the near-infrared. A slow rise of the absorption with increasing photon energies throughout the visible is followed by a sharp peak at 3.4 eV (Si) and 3.8 eV (NiO). In Si, this peak is caused by transitions from the highest valence band to the lowest conduction band along the (111) direction of the Brillouin zone. In NiO, this peak is associated with the charge-transfer gap. In both materials, the peaks broaden and redshift with increasing temperature, due to electron phonon interactions. Many recent band structure calculations for NiO focus on this main charge-transfer absorption peak (3.8 eV) and ignore the absorption below the main peak. In Si, this absorption rises smoothly (due to indirect transitions), but several peaks appear in the visible absorption of NiO, which apparently do not depend on temperature. In the infrared, the lattice absorption of Si is small because of inversion symmetry. In NiO, we find strong TO phonon absorption, which is modified by the antiferromagnetic ordering.

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