ELECTRONIC STRUCTURE, PHONON SPECTRA AND ELECTRON-PHONON INTERACTION IN TIB_2 AND ZRB_2

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The electronic structure, optical and x-ray absorption spectra, angle dependence of the cyclotron masses and extremal cross sections of the Fermi surface, phonon spectra, electron-phonon Eliashberg and transport spectral functions, temperature dependence of electrical resistivity of the MB_2 (M=Ti and Zr) diborides were investigated from first principles using the fully relativistic and full potential linear muffintin orbital methods. The calculations of the dynamic matrix were carried out within the framework of the linear response theory.

Calculated phonon spectra and phonon DOSs for both ZrB_2 and TiB_2 are in good agreement with experimental results as well as previous calculations. The Elishberg function of electron-phonon interaction in ZrB_2 is in good agreement with the experimentally measured point contact spectral function for both the position and the shape of the major peaks. We did not find regions with high electron-phonon interaction or phonon dispersion curves with soft modes in either ZrB_2 or TiB_2. This is in agreement with the fact that no trace of superconductivity was found in these borides. The averaged electron-phonon interaction constant was found to be rather small λ_{e-ph}=0.14 and 0.15 for ZrB_2 and TiB_2, respectively. We calculated the temperature dependence of the electrical resistivity in ZrB_2 and TiB_2 in the lowest-order variational approximation of the Boltzmann equation.

We found rather small anisotropical behavior of the electrical resistivity in ZrB_2 to be in good agreement with experimental observation. We found that the anisotropy of electrical resistivity in TiB_2 is larger than it is in ZrB_2.