PHONON SPECTRA AND ELECTRON-PHONON INTERACTION IN HfB_2

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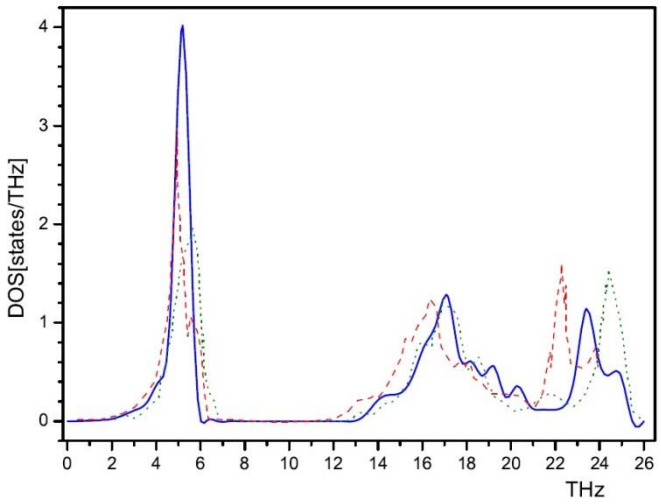
Ceramics based on transition metal borides such as HfB_2 have a unique combination of mechanical and physical properties: high melting points (>3000 °C); high thermal and electrical conductivity; chemical inertness against molten metals; great thermal shock resistance. Thus, the diboride HfB_2 is a very attractive candidates for high temperature thermomechanical structural applications up to temperatures ≈3000 °C. Potential applications include thermal protective structures for leading-edge parts on hypersonic re-entry space vehicles, propulsion systems, furnace elements,refractory crucibles and plasma-arc electrodes.



Theoretically calculated phonon density of states (full blue line) for HfB_2 .The dotted green and red dashed lines present the calculated phonon DOS of HfB2 by Deligoz [2] and Lawson [3] (VASP), respectively.

For the calculation of the phonon spectra and electron-phonon interaction a scalar relativistic FP-LMTO method [1] was used. Figure shows theoretically calculated phonon density of state for HfB_2 (full blue curve). The DOS for HfB_2 can be separated into three distinct regions. Based on our analysis of relative directions of eigenvectors for each atom in unit cell, we find that the first region (with a peak in phonon DOS at 5.2 THz) is dominated by the motion of Hf atoms. This region belongs to the acoustic phonon modes. The second wide region (14-20 THz) results from the coupled motion of Hf and the two B atoms in the unit cell. The E_{1u}, A_{2g}, B_{1g} phonon modes lie in this area. The phonon DOS in the third region extends from 22 THz to 26 THz. This is due to the movement of boron atoms and is expected since boron is lighter than Hf. The covalent character of the B-B bonding is also crucial for the high frequency of phonons. The in-plane E_{2g} mode belongs to this region. The second and third regions represent optical phonon modes in crystals. The most significant feature in the phonon DOS is a gap around 6-13 THz. This gap is a consequence of the large mass difference between B(10.8 a.u.) and Hf (178.49 a.u.), which leads to decoupling of the transition metal and boron vibrations. We compare our results with theoretically calculated phonon DOS by Deligoz et al. [2] and Lawson et al. [3]. Calculations of Deligoz et al. were based on the so-called ”frozen phonon” technique and built an optimized rhombohedral supercell with 36 atoms. This method is inconvenient for calculating phonon spectra for small q-points as well as for compounds with large number of atoms per unit cell. Lawson et al. used two different codes to calculated the phonon spectra. VASP, the supercell method, based un the projected augmented wave potentials. Second method, ABINIT, used Fritz Haber Institute pseudopotentials in the Troulliers-Martin form. VASP results of Lawson et al. is slightly closer to our calculation with respect to ABINIT data. There is an energy shift towards smaller energies of the all peaks of the Lawson et al. [3] calculations in comparison with the Deligoz et al. [2] data. Our results are just in between these two calculations.

References:

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[3] Lawson J W, Bauschlicher C W and Daw M S 2011 *J. American Ceramic Society* 94 3494