LiBC and related compounds under high pressure

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Abstract

Electronic and lattice properties of LiBC($P6_3$/mmc) and MgC_2($P6/mmm$) under a variety of compression conditions are calculated at present study. The lattice properties are optimized automatically by the first-principles molecular dynamics (FPMD) method. An anomalous lattice behaviour of LiBC under *a, b*-axis compression is found.

Key words: LiBC; Lattice anomaly; high pressure; first principles calculation

A new high-critical-temperature (T_c) intermetallic superconductor material MgB_2 (T_c = 39 K) was discovered by Nagamatsu *et al.* [1]. Many papers in experiment and theory have already been published [2]. We have calculated the electronic and lattice properties of MgB_2 and related phases under a variety of compression conditions (hydrostatic, uniaxial, *a, b*-axis) in the previous studies [3–5]. Many related compounds have already been investigated [2]. LiBC [6–9] is one of them.

The present total energy pseudopotential calculation is based on the local density approximation in the density functional theory [10,11] with the Wigner interpolation formula [12] for the exchange-correlation. The norm-conserving pseudopotentials for Li [13] and for Mg, B and C [14] are used. A partial core correction (PCC) [15] is considered for the Li and Mg pseudopotentials. The number of sampling k-points is 95 in the irreducible Brillouin zone (BZ). The details of the calculation process with the cell optimization using FPMD were reported in our previous work [3]. In addition, an all-electron calculation using the WIEN97 package [16] is performed as for LiBC with 72 k-points. Exchange-correlation type is used for the LDA form [17]. All systems maintain the crystal symmetry under compression.

The optimized lattice properties in the pseudopotential calculation are tabulated in Table 1. It is found that the lattice constant c decreases anomalously under *a, b*-axis compression Pxy = 20, 50 GPa. A contraction of the lattice constant c for LiBC is about 0.03 Å under Pxy = 50 GPa. Generally, the lattice constant c expands under *a, b*-axis compression. Therefore, this contraction implies a kind of negative Poisson ratios, even if this value (0.03 Å) is small. There is no anomalous behaviour for LiBC under *c*-axis compression and MgC_2 under *a, b*-axis compression. A deviation of lattice constants (both *a*-axis and *c*-axis) of LiBC at 95 and 259 k-points are sufficiently converged within 0.01 Å.

Table 1
Optimized lattice constants[Å] and the c/a ratios of LiBC under *c*-axis (Pz) and *a, b*-axis (Pxy) compression and MgC_2 under *a, b*-axis (Pxy) compression using the pseudopotential calculation.

	c	a	c/a
LiBC Pxy = 0 GPa	6.87	2.73	2.52
LiBC Pxy = 20 GPa	6.86	2.67	2.58
LiBC Pxy = 50 GPa	6.84	2.59	2.64
LiBC Pz = 50 GPa	5.53	2.75	2.01
LiBC Pz = 100 GPa	4.33	2.88	1.50
MgC_2 Pxy = 0 GPa	5.54	2.58	2.14
MgC_2 Pxy = 50 GPa	7.63	2.39	3.20
LiBC(Exp [18])	7.058	2.752	2.56

The anomalous behaviour of LiBC was also checked by using all-electron calculations. The lattice constants c were optimized for fixed a. The results are tabu-

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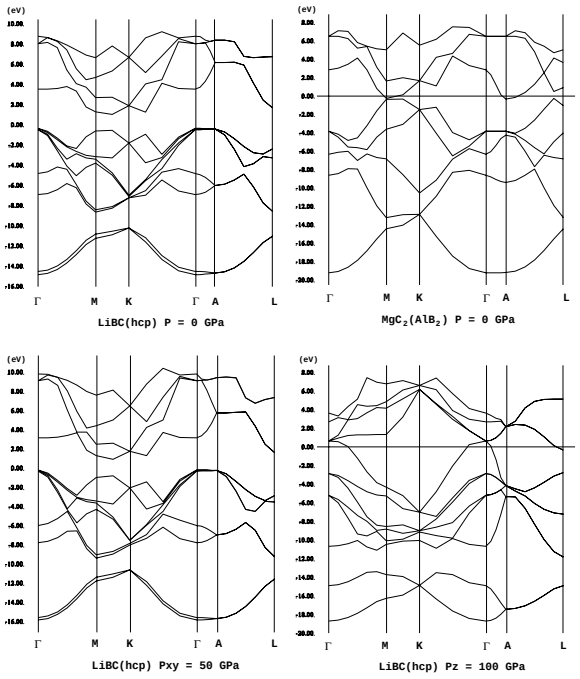

Fig. 1. The electronic band structures of LiBC (Pxy = 0, 50 GPa and Pz = 100 GPa) and MgC_2 (Pxy = 0 GPa). The Fermi level is indicated by the horizontal line.

lated in Table 2. The trend of the anomalous behaviour agrees with that using the pseudopotential calculation.

Table 2
Optimized lattice constants[Å] and the c/a ratios of LiBC using the WIEN97 [16].

	c	a	c/a
LiBC	6.828	2.725	2.51
LiBC	6.826	2.699	2.53
LiBC	6.823	2.672	2.55
LiBC	6.821	2.646	2.58
LiBC	6.822	2.619	2.60
LiBC	6.819	2.593	2.63
LiBC	6.816	2.567	2.66
LiBC	6.813	2.540	2.68

The electronic band structures of LiBC under Pxy = 0, 50 and Pz = 100 and MgC_2 under Pxy = 0 GPa are shown in Fig. 1. As for LiBC, the electronic structures under Pxy = 0, 20, 50 GPa and Pz = 50 GPa are insulator. The electronic structure of LiBC under Pz = 100 GPa is metallic. The electronic structures of MgC_2 under Pxy = 0, 50 GPa are metallic, in which a variation of the band structures is not small. The σ bands of MgC_2 are completely filled at the Γ-A line. This suggests a possibility of superconductivity could be very low.

We have calculated the electronic and lattice properties of LiBC and MgC_2 under a variety of compression conditions by using the pseudopotential and all-electron methods. We cannot find new candidates of the superconductor compounds under high pressure. We have found the anomaly of the lattice constant (c-axis) change for LiBC under *a, b*-axis compression. A more accurate and intensive study with increased k-points and energy cutoff [19] must be performed in the near future.

Acknowledgements

The numerical calculations were performed at The National Institute for Materials Science (Namiki, AlphaServer GS140 for COMPAQ).

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