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M1Po2A-04 [28]: Structure and properties of MgB₂ bulks

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It has been shown experimentally that the stoichiometry of a superconducting magnesium diboride having AlB₂ structure with a high level of superconducting properties (transition temperature to superconducting state, critical current density, upper critical magnetic field, and field of irreversibility) is close to MgB_{1.75}O_{0.25}. The ab-initio simulation confirmed the possibility of the existence of solid substitution solutions (boron to oxygen) and the energy benefit of such stoichiometry, as well as the fact that the impurity oxygen with the high probability is included in each second plane of boron of the elemental atomic cell of magnesium diboride, while every second hexagonal plane of boron of the same unite cell remains unchanged. The DFT calculations for the composition MgB_{1.75}O_{0.25} were carried out using the program packages ELK v4.3.06 –all-electron full-potential linearized augmented-plane wave (FP-LAPW) codes with exchange-correlation functionals for solids by Perdew-Burke-Ernzerhoff (PBE) in generalized gradient approximation (GGA). The k-point mesh grid was equal to 8×8×8 k-points. The manual optimization of the lattice parameters was performed by fitting the universal equation of state. The proper values of the muffin-tin radii were selected automatically at the initial stage of the calculations. $R_{\min}(\text{MT}) \times \{|G+k|\}$ was set to 7, where $R_{\min}(\text{MT})$ is the minimum muffin-tin radius used in the system. The phonon calculations (2×2×2 q-points) were performed for the optimized structure and the calculations of the superconducting critical temperature were conducted within Eliashberg theory. In order to introduce oxygen in the initial MgB₂, the symmetry was reduced and the supercell 1x1x2 along the c-axis was constructed. The calculated superconducting critical temperature T_c for MgB_{1.75}O_{0.25} is 23.3 K. Transition temperatures of the synthesized high density magnesium diboride bulks with critical current densities $J_c(0 - 1 \text{ T}, 20 \text{ K}) = 0.9 - 0.4 \text{ MA/cm}^2$ were 36-38 K.

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