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Electron-phonon coupling and superconductivity in MgB_2 under hydrostatic pressure. RAMIRO QUIJANO, FILIBERTO ORTIZ, ROMEO DE COSS, Department of Applied Physics, Cinvestav-Merida, Mexico, AARON AGUAYO, Facultad de Matemáticas, Universidad Autónoma de Yucatán, México — We have studied the dynamics and coupling of the E_{2g} phonon mode with the σ-band in MgB_2 under pressure using the Frozen Phonon Approximation. The results were obtained by means of first-principles total-energy calculations using the full potential Linearized Augmented Plane Wave (LAPW) method and the Generalized Gradient Approximation (GGA) for the exchange-correlation potential. We present results for the evolution of the anharmonicity and phonon frequency of the E_{2g} mode, the electron-phonon coupling constant, and T_c as a function of hydrostatic pressure in the range 0-40 GPa. We find that the phonon frequency increases monotonically with pressure, but the the anharmonicity, the electron-phonon coupling and T_c decreases with pressure. We have obtained a very good agreement between the calculated $T_c(P)$ and the experimental data available in the literature, in particular with the experimental data corresponding to monocystalline samples. This work was supported by Consejo Nacional de Ciencia y Tecnología (CONACYT, México) under Grant No. 43830-F.

Romeo de Coss
Department of Applied Physics, Cinvestav-Merida, Mexico.

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