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Properties from spin-phonon coupling in high-T_C superconductors: $HgBa_2CuO_4$ and $La_{(2-x)}Sr_xCuO_4$ THOMAS JARLBORG, DPMC, University of Geneva, Switzerland — The mechanism of spin-phonon coupling (SPC) in high-T_C copper oxides is explored from band calculations on LSCO and HBCO systems. The LMTO band calculations, based on the local density approximation, are made for cells containing frozen phonon displacements and/or spin waves within the CuO plane. The virtual crystal approximation is used for studies of hole doped systems. The main result is that phonons are favorable for spin waves and vice-versa, and that pseudogaps appear naturally in the band structures of striped materials with strong SPC. The wave length of the spin-phonon modulation is related to doping, and the mutual enhancement of SPC is strongest when the non-doped system is close to an anti-ferro magnetic ground state. The calculated band results are used for modelling of different properties, such as isotope effects, phonon softening, shear dependences and T-variations. The results are discussed and compared with experiment. It is speculated that perpendicular SPC, with different behavior along x- and y-directions, can produce double gap structures. A moderate correction to LDA, which stabilizes the AFM state for the undoped material, will enhance the coupling constant for spin fluctuations λ_{sf} for doped cases. These results suggest that properties of high-T_C superconductors should depend both on phonons and magnetic fluctuations.

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