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Surface-induced reduction of the spin coherence times of nitrogen-vacancy centers in diamond JEFFREY M. MOORE, MICHAEL E. FLATTÉ, Department of Physics and Astronomy, University of Iowa — The exceptionally long room-temperature spin coherence times of nitrogen-vacancy (NV) centers in diamond indicate their potential utility for quantum information processing. The remarkable sensitivity of the spin dynamics of NV centers to electric and magnetic fields, and to strain, also suggests these centers can be used in novel sensors. The sensitivity and spatial resolution of such a sensor will depend on the depth of the NV center below the diamond surface. Local relaxation of the atomic positions near the diamond surface, however, will strain the NV center and consequently reduce its spin coherence time. We evaluate this effect by calculating the strain near a (001) diamond surface using density functional theory. The strain for a specific NV-center depth was evaluated using the linearized augmented plane wave (LAPW) method and the Perdew-Burke-Ernzerhof (PBE) exchange correlation functional within the WIEN2k density functional code. The effect of the resulting strain values on the spin coherence times were determined using a low-energy effective Hamiltonian for the NV-center energies and wave functions, and their strain dependence. This work was supported by an AFOSR MURI.

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