Abstract

Quantum computers (QC), if realized, can overwhelm the performance of conventional computers in a number of calculational tasks. A hydrogenic donor in silicon is one of the most promising candidates as a fundamental building block of QC referred to as a quantum bit (qubit) towards realization of future solid-state QC. Application of donors as qubits requires in-depth understanding of their structural, electronic, and magnetic properties. Moreover, control of their interactions with nuclear spins in silicon matrix is needed.

The present thesis reports investigations of magnetic properties of lithium (Li) hydrogenic donor related centers in silicon by electron paramagnetic resonance (EPR) spectroscopy and dynamic nuclear polarization (DNP) of host ^{29}Si using lithium related centers in isotopically controlled silicon. Lithium is the only non-substitutional hydrogenic donor in silicon that forms a complex pair with an oxygen atom very easily. Thanks to its low ionization energy and inverted ground state energy levels, long electronic spin decoherence time (T_2) and short electron relaxation time (T_1) that are favorable for construction of QC are expected.

The present thesis is composed of six chapters. Chapter 1 is an introduction and 2 provides a literature survey on lithium related centers in silicon. Chapter 3 provides basic principles of magnetic resonance. Chapter 4 discusses EPR of lithium related center in silicon. Significant narrowing of the isolated Li EPR and additional hyperfine structures of lithium-oxygen (Li-O) centers were observed in isotopically enriched ^{28}Si single crystals. Unexpected splitting was found reflecting the principal axis of the formally assigned trigonal *g*-tensor being 3^{o} tilted from <111> crystal axis, i.e., the g-tensor of the Li-O center actually has a monoclinic symmetry. Furthermore splitting of ^{7}Li hyperfine lines into four components was observed at temperatures 3.5 K. These findings provided accurate knowledge of EPR frequencies of Li related centers that are needed for high fidelity operation of Li quantum bits in silicon. Chapter 5 reports dynamic nuclear polarization (DNP) of ^{29}Si nuclear spins induced by saturation of EPR transitions of lithium-related centers. Both isolated Li and Li-O complex centers showed strong EPR absorption lines in the temperature range 3.4-10 K and led to very efficient orientation of

^{29}Si nuclear spins. The temperature dependence and time constant of ^{29}Si DNP are investigated in detail. The ^{29}Si DNP of 0.72 % was achieved at 3.4 K by excitation of the Li-O forbidden EPR transition under illumination, corresponding to a ~352 fold increase with respect to the thermal equilibrium polarization. Possible strategies are discussed to obtain >5% ^{29}Si DNP that is needed for realization of quantum computing. Chapter 6 provides conclusions and outlook.