Characterization of the xenon polarization process and comparison with theoretical predictions

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Introduction

The production of hyperpolarized xenon is of current interest for medical imaging and materials science, and a number of different approaches have been proposed for obtaining the large quantities of gas and high level of polarization needed for these applications. Xenon polarization through spin-exchange with optically pumped Rb vapour (OPSE) is a method widely used by the HpXe community around the world, and over the past 20 years Happer and co-workers studied in depth the physics that regulates the build-up of xenon polarization with this approach [1].

However, balancing tradeoffs of noble gas polarization, production rates, volumes, and magnetization involves exploring a large parameter space, and there still exists some uncertainty regarding the optimal choice of parameters to maximize the Xenon polarization.

We implemented the current theoretical knowledge of the spin-exchange process into a numerical simulation, and using our experimental polarizer we measured the gas polarization varying several parameters in order to test the validity of our theoretical predictions.

Numerical simulations: methods

The numerical simulation of the polarization process was implemented in Matlab (TheMathWorks). The level of Rb polarization was calculated by solving a nonlinear system of equations that included the effects of: laser beam profile and power, temperature dependence of Rb density, effect of skew light propagation, shape and dimensions of the optical cell, pressure broadening and pressure shift of the Rb absorption line, whereas diffusion of Rb atoms inside the optical cell and Rb wall relaxation effects were neglected.

The binary collision and van der Waals molecules contribution to the ^{129}Xe-Rb spin exchange rate was considered given by

$$\gamma_{se} = [Rb]\left(\langle\sigma_{se}\upsilon\rangle + \frac{\zeta_{Rb}}{\gamma^{-1}_{Xe-mol}[Xe]+\gamma^{-1}_{N_2-mol}[N_2]+\gamma^{-1}_{He-mol}[He]}\right)$$

where [Rb] is the number density of Rb, [Xe], $[N_2]$ and [He] are the number densities of all gases present in the mixture, $\langle\sigma_{se}\upsilon\rangle$ is the velocity averaged binary spin exchange cross section, ζ_{Rb} is a constant which depends on the nuclear spin and relative abundance of each isotope of Rb, and $\gamma_{gas-mol}$ are the molecular spin exchange rates associated with third body gases Xenon, Nitrogen and Helium.

Results of the numerical simulations are shown in Figure 1-6 for different values of optical pumping parameters (temperature, pressure, laser power, etc.). In the different graphs we report the average level of ^{129}Xe polarization inside the optical cell.

^{129}Xe polarization measurements: methods

Hyperpolarized xenon was produced by optical pumping and spin exchange using the method described by Driehuys *et al*. [2]. A mixture of 1% 129Xe, 1% N2 and 98% He, was loaded into an optical cell containing a visible drop of rubidium. The Rb vapour was optically pumped with circularly polarized light from a 100 W diode laser array (OptoPower). The level of ^{129}Xe polarization was measured with a NMR apparatus (Resonance Instruments) operating at 150 kHz. The absolute polarization of the gas was obtained by comparing the HpXe signal with the proton signal obtained from an equivalent cell filled with a known quantity of water doped with gadolinium. The water signal was averaged over 10000 scans, while the gas signal was averaged over 16 scans.

The level of average Rb polarization inside the optical cell was obtained from the difference between the optical spectra transmitted through the cell with and without the magnetic field generated by the Helmoltz coils.

Numerical simulations: results

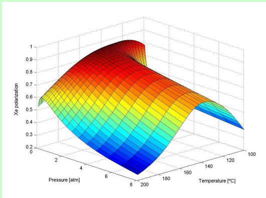

Figure 1

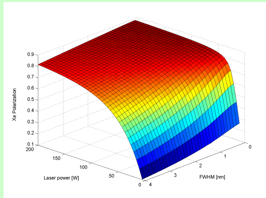

Figure 2

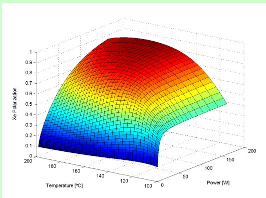

Figure 3

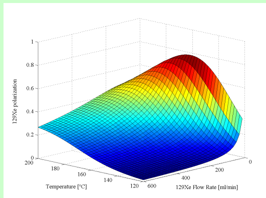

Figure 4

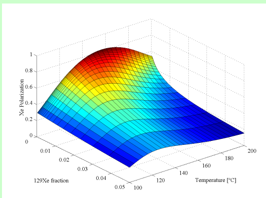

Figure 5

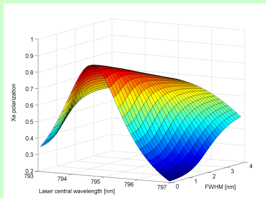

Figure 6

^{129}Xe polarization measurements: results

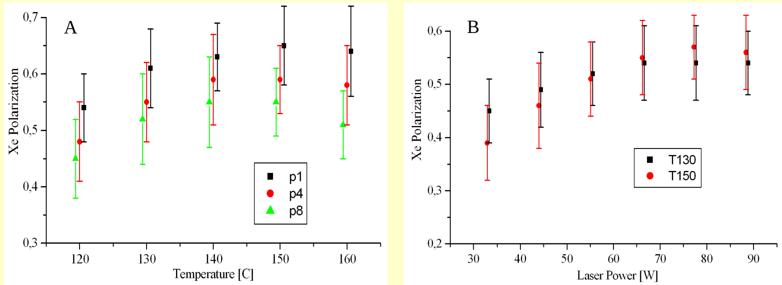

Figure 7. (A) Measured Xe polarization vs cell temperature for different pressures of the gas mixture (1.2 Atm, 4.6 Atm, 8.0 Atm); (B) Xe polarization vs laser power at two temperatures (130℃, 150 ℃)

Discussion and conclusions

Theoretical simulation and experimental measurements of xenon polarization show common features. For a fixed pressure, we observe that there is an optimal temperature that maximizes the xenon polarization (Fig 1, Fig. 7a). Moreover, increasing the laser power over a certain threshold that depends on the temperature does not increase the total xenon polarization (Fig. 3, Fig. 7b). These effects are a result of the combined characteristics of the optical cell dimensions and of the laser beam. Laser with a narrower width do produce higher Xenon polarizations, but the tuning of the central wavelength becomes critical (Fig. 6).

We observed that by lowering the total gas pressure the level of xenon polarization increases, with a maximum polarization when the contribution to Xe-Rb spin-exchange from van der Waals molecules as calculated from the simulation becomes about equal to the contribution from the binary collision term (Fig. 8).

Although some of these results were observed by other groups [3-5], they were not analyzed systematically before. We believe that these observations should be taken into account for the design of new xenon polarizers using optical pumping and spin exchange, and could be helpful for the interpretation of published results [3-5].

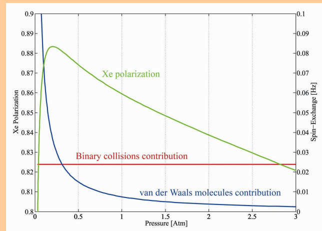

Figure 8. Xe polarization and spin-exchange terms at 150 ℃ vs total gas pressure

References

[1] TG Walker and W Happer, Rev Mod Phys, (1997) 69, 629. [2] B Driehuys et al., Appl Phys Lett, (1996) 69, 1668. [3] AL Zook et al., JMR, (2002) 159, 175. [4] NJ Shah et al., NMR Biomed., (2000) 13, 214. [5] IC Ruset and FW Hersman, 45th ENC conference, (2003).

Acknowledgments

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