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Comparative analysis of two methods of laser induced boron isotopes separation

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Natural boron consists of two stable isotopes 10B and 11B with natural abundance of 18.8 atom percent of 10B and 81.2 atom percent of 11B. The thermal neutron absorption cross-section for 10B and 11B are 3837 barn and 0.005 barn respectively. 10B enriched specific compounds are used for control rods and as a reactor coolant additives.

In this work 2 methods for boron enrichment were analysed:

1) Gas irradiation in static conditions. Dissociation occurs due to multiphoton absorption by specific isotopes in appropriately tuned laser field. IR shifted laser pulses are usually used in combination with increasing the laser intensity also improves selectivity up to some degree. In order to prevent recombination of dissociated molecules BCl3 is mixed with H2S

2) SILARC method. Advantages of this method:

a) Gas cooling is helpful to split and shrink boron isotopes absorption bands. In order to achieve better selectivity BCl3 gas has to be substantially rarefied (～0.01%-5%) in mixture with carrier gas.

b) Laser intensity is lower than in the first method.

Some preliminary calculations of dissociation and recombination with carrier gas molecules energetics for both methods will be demonstrated

Boron separation in SILARC method can be represented as multistage process:

1) Mixture of BCl3 with carrier gas is putted in reservoir

2) Gas overcooling due to expansion through Laval nozzle

3) IR multiphoton absorption by gas irradiated by specifically tuned laser field with subsequent gradual gas condensation in outlet chamber

It is planned to develop software which includes these stages. This software will rely on the following available software based on quantum molecular dynamics in external quantized field:

1) WavePacket: Each particle is treated semiclassicaly based on Wigner transform method

2) Turbomole: It is based on local density methods like density of functional methods (DFT) and its improvement- coupled clusters approach (CC) to take into account quantum correlation.

These models will be used to extract information concerning kinetic coefficients, and their dependence on applied external field. Information on radiative corrections to equation of state induced by laser field which take into account possible phase transition (or crossover?) can be also revealed. This mixed phase equation of state with quantum corrections will be further used in hydrodynamical simulations. Moreover results of these hydrodynamical simulations can be compared with results of CFD calculations. The first reasonable question to ask before starting the CFD simulations is whether turbulent effects are significant or not, and how to model turbulence?

The questions of laser beam parameters and outlet chamber geometry which are most optimal to make all gas volume irradiated is also discussed. Relationship between enrichment factor and stagnation pressure and temperature based on experimental data is also reported.

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