Neutron and X-ray Structural Investigations of Liquid Oxides

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NEUTRONS FOR SCIENCE

Student CLIP Session 2005

CNRS CENTRE NATIONAL DE LA RECHERCHE SCIENTIFIQUE

Motivation

What we want to do...

1. Local structure study of atomic arrangement in the liquids at short and intermediate range
2. Development of Aerodynamic Levitation system combined with Laser Heating
3. Improve of knowledge about the physical and technological features of materials at high temperature

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Combining Neutrons and X-rays techniques we will obtain a detailed structural analysis of liquids properties

Molecular Dynamics Simulation at C-Lab at ILL

- *Ab-initio* by VASP
- Classical MD by nMoldyn

Approach

- We analyze the total structure factor $S(q)$ and the pair correlation function $g(r)$
- We calculate the coordination number $\mathcal{N}$ and atoms distances

Expressions

$$g(r) - 1 = \frac{1}{2\pi^2 \rho_0 r} \int_0^\infty q[S(q) - 1] \sin(qr) dr$$

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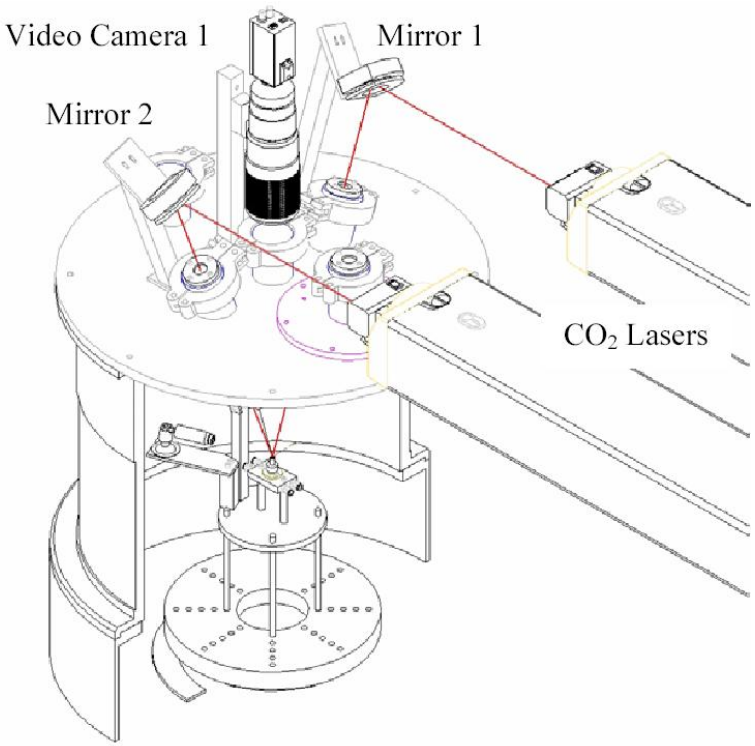
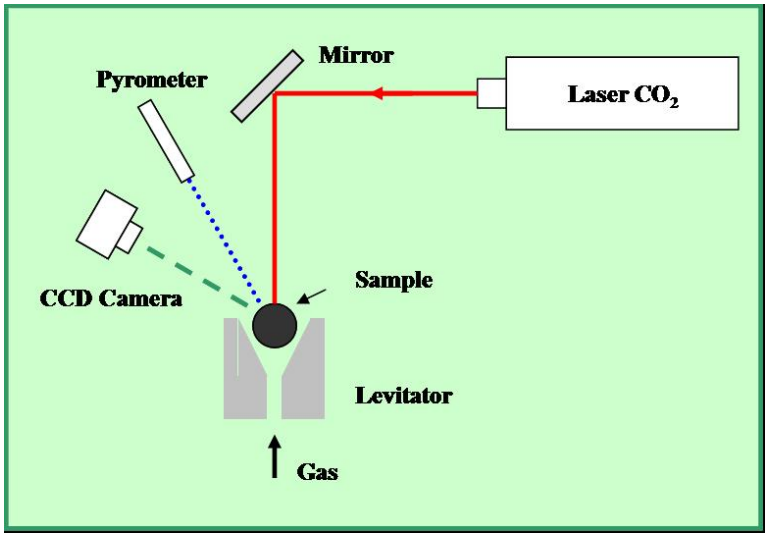
By multi-techniques approach we have reliable coordination numbers and distances in the liquid state

Levitation Tool - D4c Installation

D4c Installation at ILL





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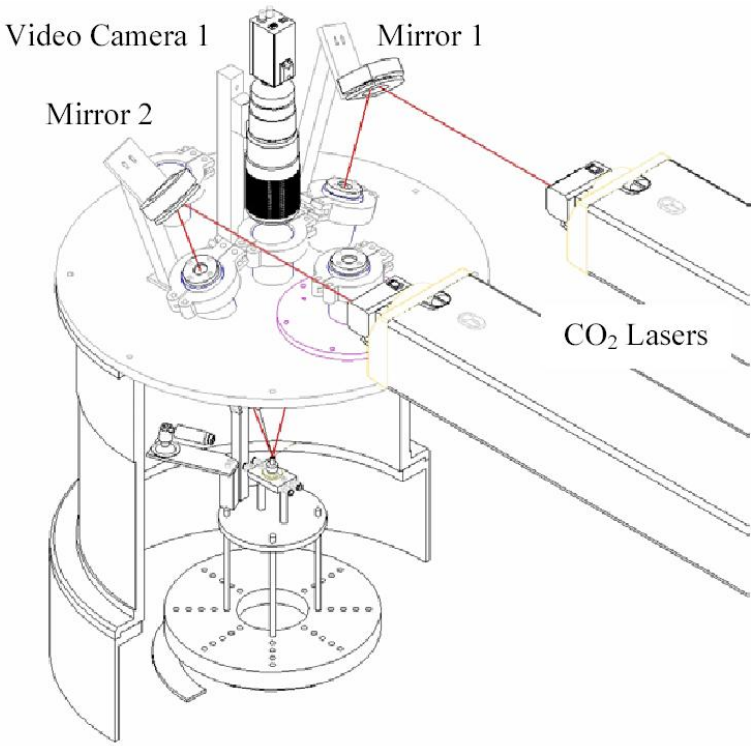
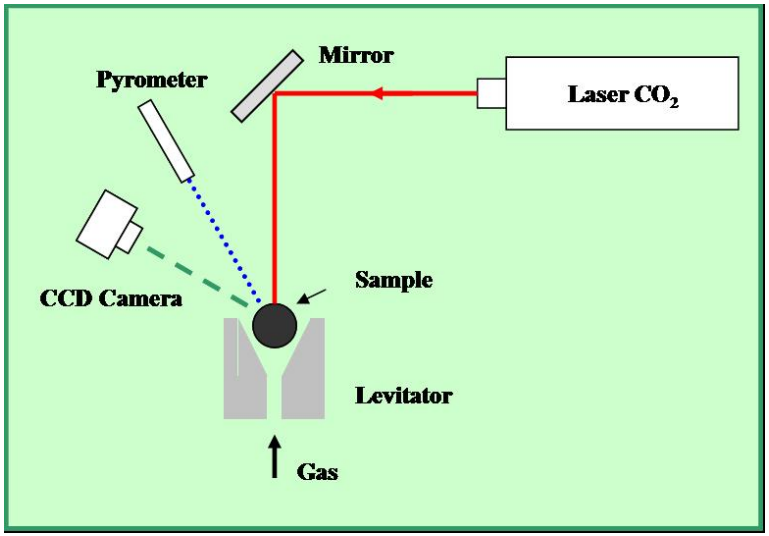
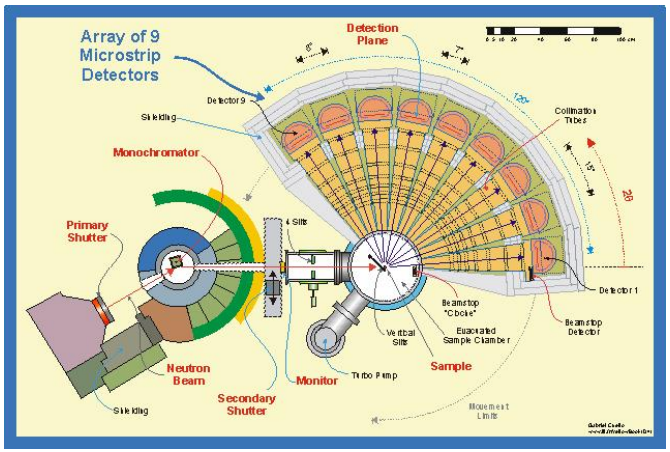
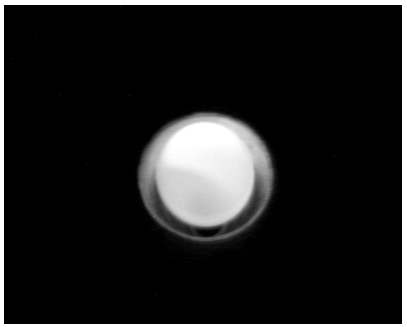
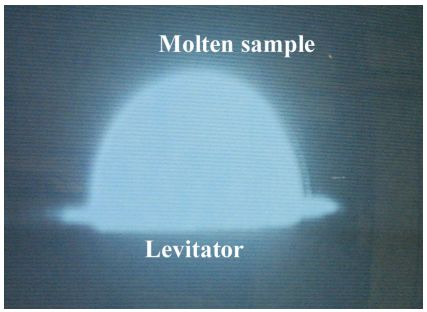






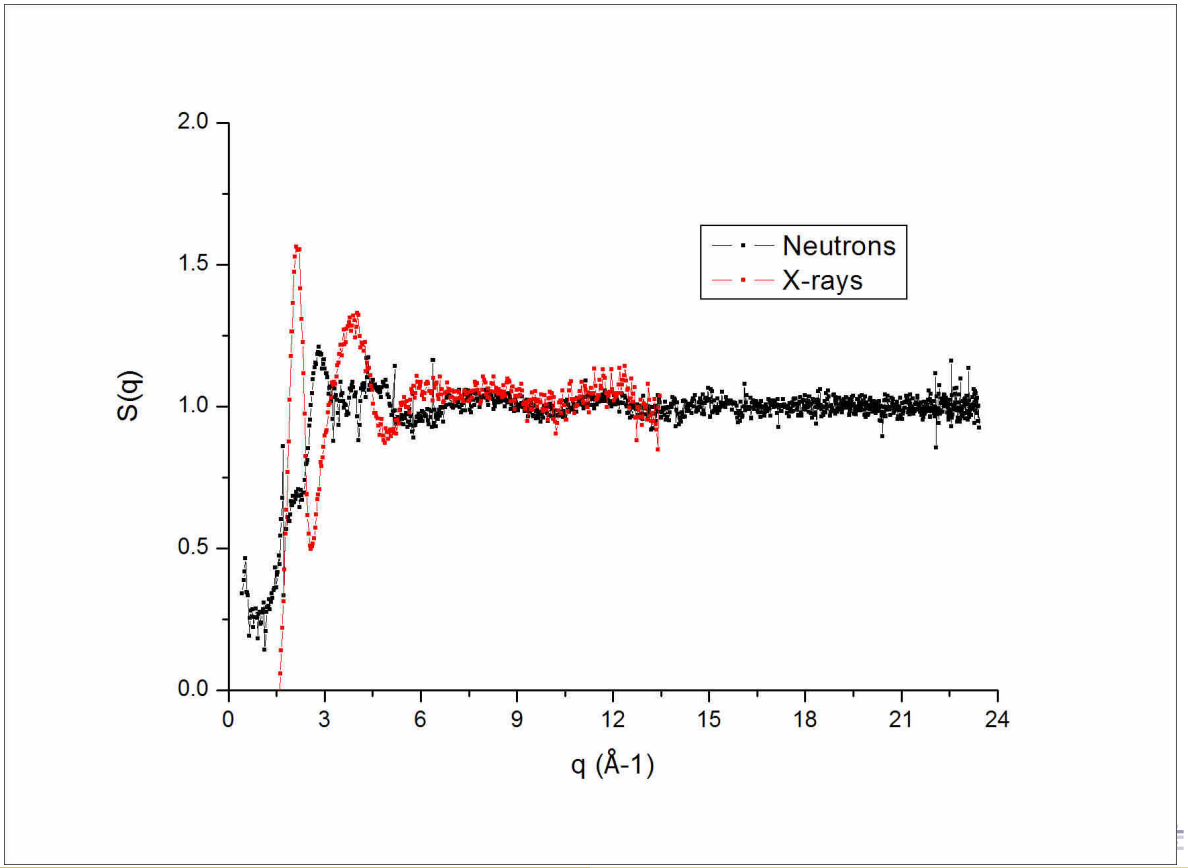




Garnet YAG, $Y_3Al_5O_{12}$ at 2100K

Laser material, optical lens, and thermal barrier coating

Neutron and X-ray diffraction data taken at D4c (ILL) and ID15 (ESRF)

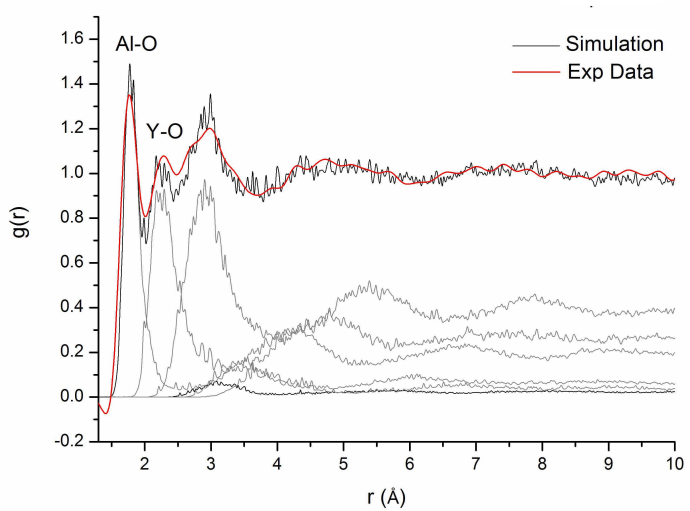


Results

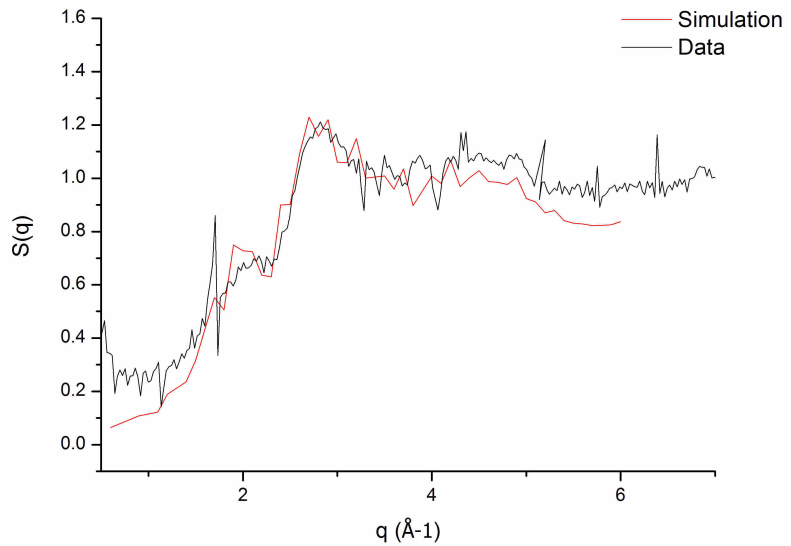
Garnet YAG, $Y_3Al_5O_{12}$ at 2100K

Laser material, optical lens, and thermal barrier coating

Ab-initio Simulation - VASP



Classical MD Simulation- nMoldyn



For the future...

MA systems, $MgAl_2O_4$ - $Mg_3Al_2O_6$ - $MgAl_4O_7$

Important component of Earth's mantle, ceramics industries fabrication

CA systems, $CaAl_2O_4$ - $Ca_3Al_2O_6$ - $CaAl_4O_7$

Ceramics industries fabrication

Silicon based Alloys, SiGe, SiC, Si_3N_4

Useful in semiconductor industry, nuclear gas-cooled fast reactor, engine components and cutting tools, very interesting for electronic applications

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