

# *Progress in the simulation of short wavelength sources during the 5 years of COST Action MP0601*

- Use of available academic / commercial software*
- Writing / upgrading simulation software*
- Writing of basic equations to describe new phenomena*

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Writing of

Simulation for design of X-ray and EUV optics

Integrated simulations of EUV-XUV sources / Description of the various types of sources : HHG, X-ray lasers, laser produced plasma sources (LPP), discharge produced plasma sources (DPP), accelerated electron sources

More fundamental atomic / plasma physics to describe specific problems and feed integrated codes

Some statistics of the Working Group 1 (WG1) :

- ~ 73 oral talks and posters in 5 years  
(can be also double-counted in other working groups)
  
- 35 people involved partly or fully dedicated to simulations  
(6 women, 29 men)  
2/3<sup>rd</sup> Post Graduate and Early Stage Researchers (ESR)
  
- + 2 / 3 invited talks by japanese researchers
  
  
- ~ 20 oral talks and posters on simulation of optics / thermal load /  
software for image analysis
  
- ~ 20 oral talks and posters on basic atomic and plasma physics
  
- ~ 35 oral talks and posters on integrated simulations of EUV / XUV sources

## **Simulation and design of EUV / XUV optics :**

Much of the software already written for and by the synchrotron community

**SKL ray tracing program** developed with EU grant GRD1 / COST P7 support presented to the whole community. Designed to help developing EUV / XUV optics with a user friendly interface  
--> new V-shaped Ge monochromator conceived. Different geometries : V, W, cylindrical shapes  
Aberration reduction and heat load also taken into account to optimize focusing.

Ray-tracing analysis to reconstruct lasers wavefront.

Software for **imaging analysis** in order to replace lenses where they are not available has been presented. For XUV wavelengths, few lenses and difficult to manufacture.  
--> reconstruct the phase of focused light and image of an object through modulation of outgoing intensities if the XUV radiation is coherent.  
-->Modelling of harmonic propagation in a capillary : possible to filter out a single harmonic of "narrow" bandwidth. The reconstruction of the resulting images leads to 90nm resolution.

Simulation of **waveguides** to create laterally periodic waves and structures with laboratory sources. Enhancement of collimation and focusing. Computation of Talbot effect

## Simulation and design of EUV / XUV optics :

### Simulation of **Reflexion Zone** plates

Both numerical and analytical resolution

Simulations for **direct laser patterning with** two, three or four **lasers beams interfering**. Intensity distribution shows possible patterning sizes down to a few nanometers.

Simulation of **thermal load** of cathode X-ray sources. Application of synthetic diamond leads to better cooling of the anode and reduction of the thermomechanical stress.

Modelling and simulation of **Field-emitted Carbon NanoTubes (CNT) Discharge sources**.

--> Higher electrical conductivity, stability in temperature, larger field enhancement factor and lower threshold fields than conventional cathode emitters. For best efficiency, nanotubes should have uniform orientation and distribution.

## **Integrated simulations of EUV / XUV sources**

Intensive simulation work conducted on **EUV sources for nanolithography** with the **Z\*** code or Indigenous codes for both discharge- and laser-plasma based sources. Computation of optimum laser and density conditions. 1.5 % maximum conversion efficiency calculated for Xenon, 3 to 6% for Tin. Computation of integrated, time-resolved and orientation-dependant spectra. 80 to 90% conversion efficiency can be reached from laser to overall EUV light within 10-15% Bandwidth

**ARWEN** : new 2D hydro-radiative code with Adaptive Mesh Refinement (AMR)  
--> study of the edges of soft **X-ray lasing** plasmas. Edges are 70 to 80  $\mu$  wide, -> plasmas with less than 150  $\mu$  transverse focus have strong transverse gradients and poor transport / amplification of the lasing light. Simulations with 1mm transverse focus : very homogeneous and stable electron density and temperature. Gain can be optimised and stay constant over 900  $\mu$ . Increasing further the width leads to transverse lasing and saturation, preventing optimum lasing in the longitudinal direction.

**EHYBRID** to test the influence of prepulses and grazing Incidence schemes (GRIP) on X-ray lasers. Use of two short main pulses lead to a better gain in the active medium.

2D and 3D simulation tools developped for **High Harmonics Generation (HHG)**. Phase matching is increased with loose focusing and for given lower focusing by a gas pressure optimisation. Laser field is strongly affected by its propagation in the gas.

## **More fundamental computations for XUV / EUV sources**

### **Nanolithography EUV sources :**

study of influence of fast electrons on the ionisation and emissivity of Xe and Sn. Low proportion of **fast electrons** (1 to 2% at 3 KeV when the rest of the distribution is between 30 and 60 eV) swift the ionization from 11+ to 19+ at 40eV,  $10^{17}$  e-/cc while the emissivity is increased by orders around 13.5 nm. Satellite lines from Xenon 20+ to 23+ overpass the conventional emissivity of 10+ ions. This allows to account for unexplained features in experimental spectra --> more efficient EUV Xenon sources even brighter than Tin sources.

Inclusion of **configuration interaction** in the computation of **satellite lines** strongly increases the emission of Tin laser sources or modifies the optimum conditions for Xenon sources.

**Wavelength** study of various High Z emitters : **Terbium and Gadolinium** will be best at 6.x nm for the next generation EUV sources. More than 6% efficiency reachable in 0.6% bandwidth

Hydrodynamics :

Writing of a multifluid code simulating the collision of plasmas.

## **More fundamental computations for XUV / EUV sources**

### **X-ray lasers :**

new model for fast ionisation implemented in a 2D hydro radiative code ARWEN.

-->much higher plasma temperatures and proves that transient ionisation can not be postprocessed in X-ray lasers simulations.

Computation of NLTE opacity datafiles

-->LTE emissivities lead to overestimate by orders radiative cooling of X-ray lasers.

Study of effects of travelling wave speed.

Maxwell-Bloch model to compute spatial and temporal coherence of X-ray lasers

--> simulation of High Harmonic seeding and amplification in a lasing plasma. Reduction of the non-coherent amplification and of the duration of the lasing.

### **High Harmonics Generation (HHG).**

Simulations try to improve the phase matching using the full quantum model by Lewenstein.

Phase matching only due to short electron trajectories. In water window, phase matching only occurs in a limited range of half optical cycles and is thus time dependant.



Available software :

TDFEA - the program tool for thermodynamical finite element analysis

Raytracing routine for reflexion zone plate

RAY raytracing program from Bessy

FEA (Finite Element analysis) and ray-tracing of X-ray optics elements :

computation of adaptative optics / aberration effects

SKL Ray-tracing program

MultiLayer Mirrors design codes (COMSOL, ZEMAX)

Thermal load codes

X-TRACT for phase-contrast tomography

Many codes for atomic and plasma physics presented on **Plasma Gate** Weizmann :

<http://plasma-gate.weizmann.ac.il/directories/free-software/>

## Available software :

### Atomic physics :

- **FAC** (complete atomic suite with structure, energies, cross sections), very stable and easy to use, available on the web
- **HULLAC09** (complete atomic suite) very accurate energies, available on request
- **MCDF / MCHF** (complete atomic suite) very accurate energies, more tricky to use
- **COWAN CODE** (complete atomic suite) very accurate energies, also a web version with very easy interface to compute line energies, rates ...with shifts to cope with experimental results
- **FLYCHK** (complete atomic suite + population solver, LTE / NLTE / Time and radiative dependant + spectral tracer) moderately accurate but very fast and stable. Available on request
- **PrismSpect** (atomic suite + LTE / NLTE / Time and radiative dependant spectra). Low Z elements, easy to use. Commercial

### Hydrodynamics :

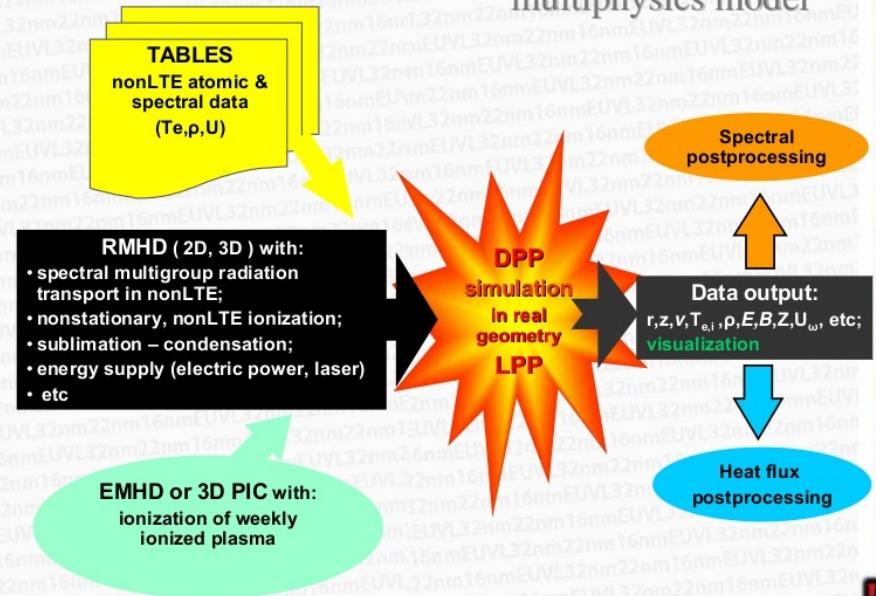
- **MULTI** 1D / 2D available on the web
- **EHYBRID** (1.5D) with atomic physics to compute X-ray laser time-dependant gain, available on request
- **ARWEN** (2D with Adaptive Mesh Refinement, radiation transport and time-dependancy) available on request, created by the DENIM team (Madrid)

### Integrated : atomic + plasma + hydro + spectra :

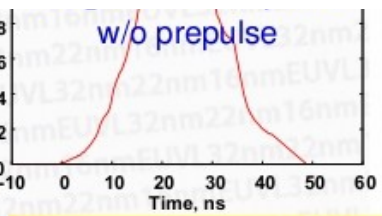
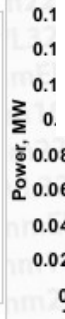
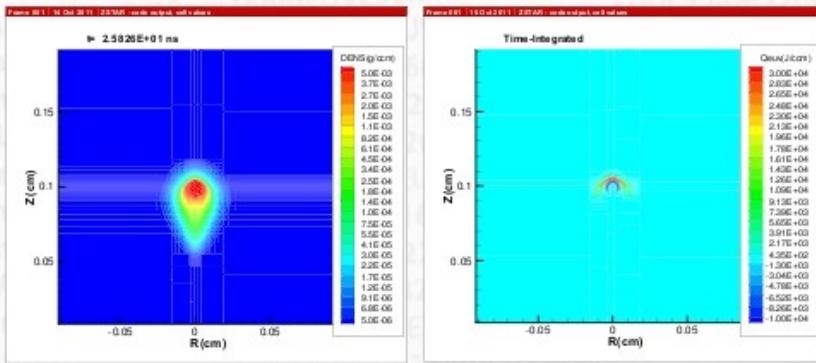
- **Zstar** : developed especially to model EUV / XUV sources by people from COST MP0601, widely used in the community (easy). Commercial

**Z\*** : developed by EPPRA / nano UV  
 Peter Choi /  
 Vasily Zakharov /  
 Sergei Zakharov

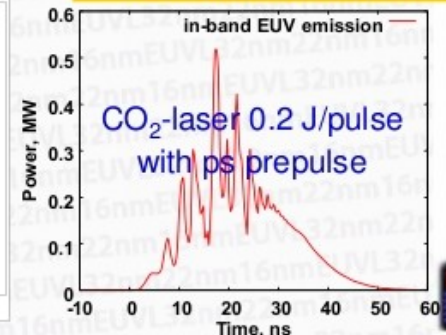
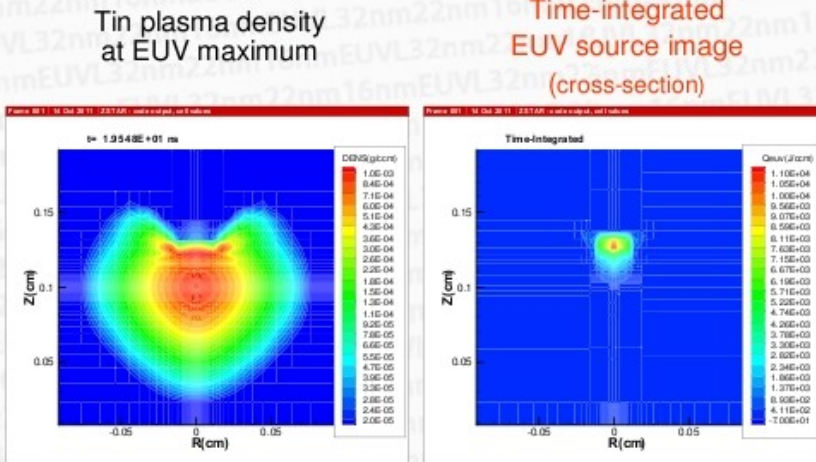
ZETA → Z\* RMHD Code → Z\* BME → Z+  
 multiphysics model



**LPP EUV Source**  
 under CO<sub>2</sub>- laser



**The maximum EUV brightness is up to 15 W/mm<sup>2</sup> sr kHz**



**in-band EUV emission**  
 CO<sub>2</sub>-laser 0.2 J/pulse with ps prepulse





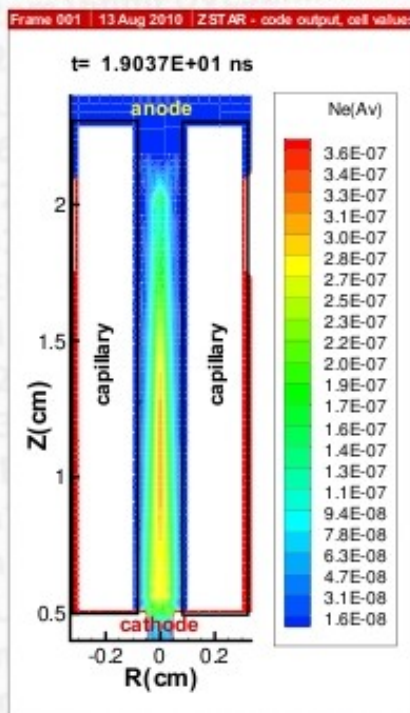
Z\* : developed by EPPRA / nano UV

Peter Choi / Vasily Zakharov / Sergei Zakharov

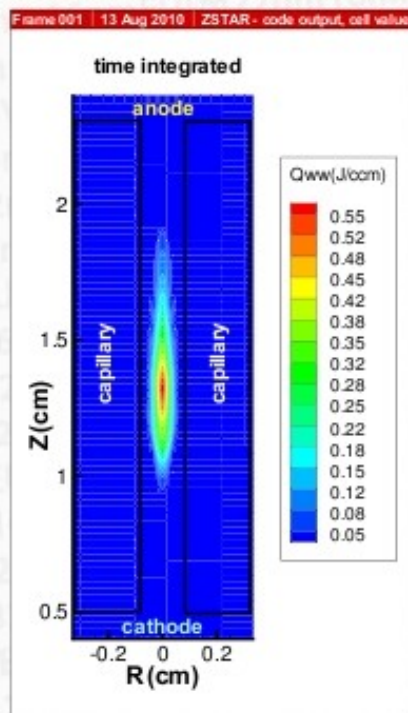
# MPP source for soft x-ray microscopy

## Z\*-code modelling

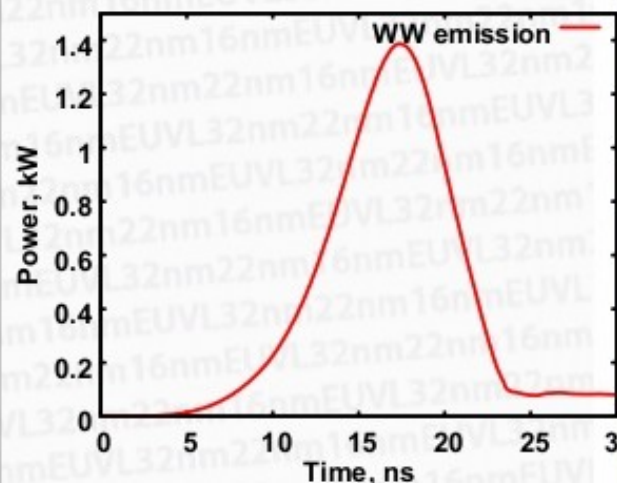
Nitrogen plasma  
near emission maximum



Time integrated image of  
soft x-ray (426.5 - 431eV) source



Soft x-ray pulse  
in 0.01nm band @ 2.8817nm



Nitrogen: He-like and H-like

0.48J/pulse charge

Fast electrons induce  
discharge in 3-D  
volumetric compression  
regime

$\langle Z \rangle \approx 4-5$

$T_e = 45 - 55 \text{ eV}$

$n_e \approx 2 \cdot 10^{17} \text{ cm}^{-3}$



2011  
International  
Workshop  
on EUV and  
Soft X-Ray  
Sources

Nov 7-10  
Dublin  
Ireland

## Networking

Shared codes :

SKL for optics design (shared knowledge)

Z\* (code + people sharing for development on site)

FAC (shared knowledge on use)

HULLAC (shared knowledge on use)

ARWEN (shared knowledge on use, adaptation of the code)

School for graduate european students on EUV sources in Dublin (may 2010)

Teaching by some COST members, access to graduate students from the COST

## Acknowledgement of the COST action MP0601

X-ray laser conferences

EUV nanolithography conferences

Radiative Properties of Hot Dense Matter (RPHDM) conferences

Inertial Fusion Science and Applications (IFSA) conference

Non Local Thermodynamic Equilibrium (NLTE) workshops

Thank you !!

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