

# Simulation on charge states evolution of XFEL heated target

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## Introduction

Since X-ray Free-Electron Lasers (XFELs) opens up new regimes in x-ray—matter interactions, there have been several discoveries of nonlinear optical phenomena in the soft and hard X-ray regions at XFEL facilities. One of the interesting phenomena is the initial phase of transformation of solid density aluminum plasma by analyzing time-resolved extreme ultraviolet (XUV) absorption spectroscopy with a time resolution of 10 fs or less. The material state is produced with XFEL via K-shell photo-absorption and probed by a few fs XUV pulses at various delays. XUV absorption edges are directly related to ionization energies of core electrons (ex. Al L-level) and electron distributions at the continuum. In order to verify the mechanism, XFEL heating is modeled using the collisional-population kinetic code SCFLY. We calculate the temporal evolution of charge states and temperature of 200 nm aluminum irradiated with 5 keV XFEL pulse of 10 fs duration. This calculation could show the ultrafast dynamics of inner-shell electrons, and electron thermalization during intense XFEL – matter interaction.

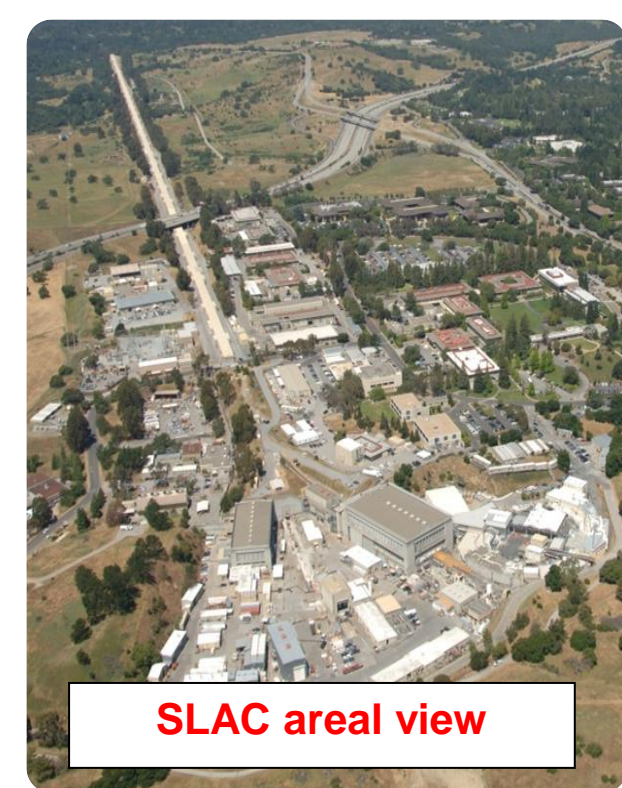
## Simulation code and condition

### Simulation Code SCFLY Ver 1.9

- A collisional radiative simulation code based on the FLYCHK.
- Population distribution is obtained by rate equation considering collisional and radiative atomic processes.
- Providing a spectrum of light-matter interaction, ionization and population distribution of plasma.



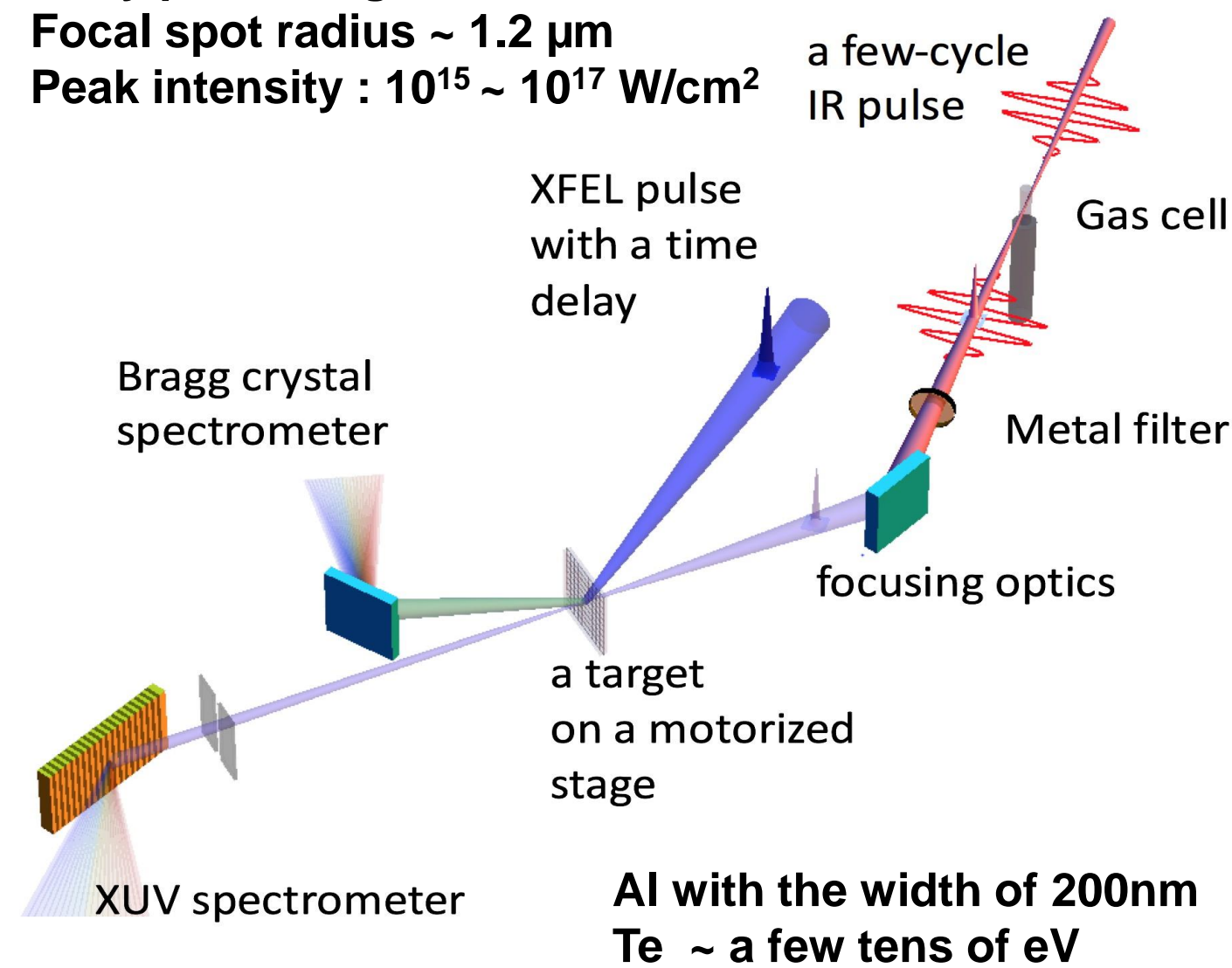
### Simulation condition



#### XFEL Character in LCLS

- X-ray photon energy : 5000 eV
- X-ray pulse length ~ 10 fs
- Focal spot radius ~ 1.2 μm
- Peak intensity : 10<sup>15</sup> ~ 10<sup>17</sup> W/cm<sup>2</sup>

Peak intensity  
10<sup>16</sup> ~ 10<sup>17</sup> W/cm<sup>2</sup>

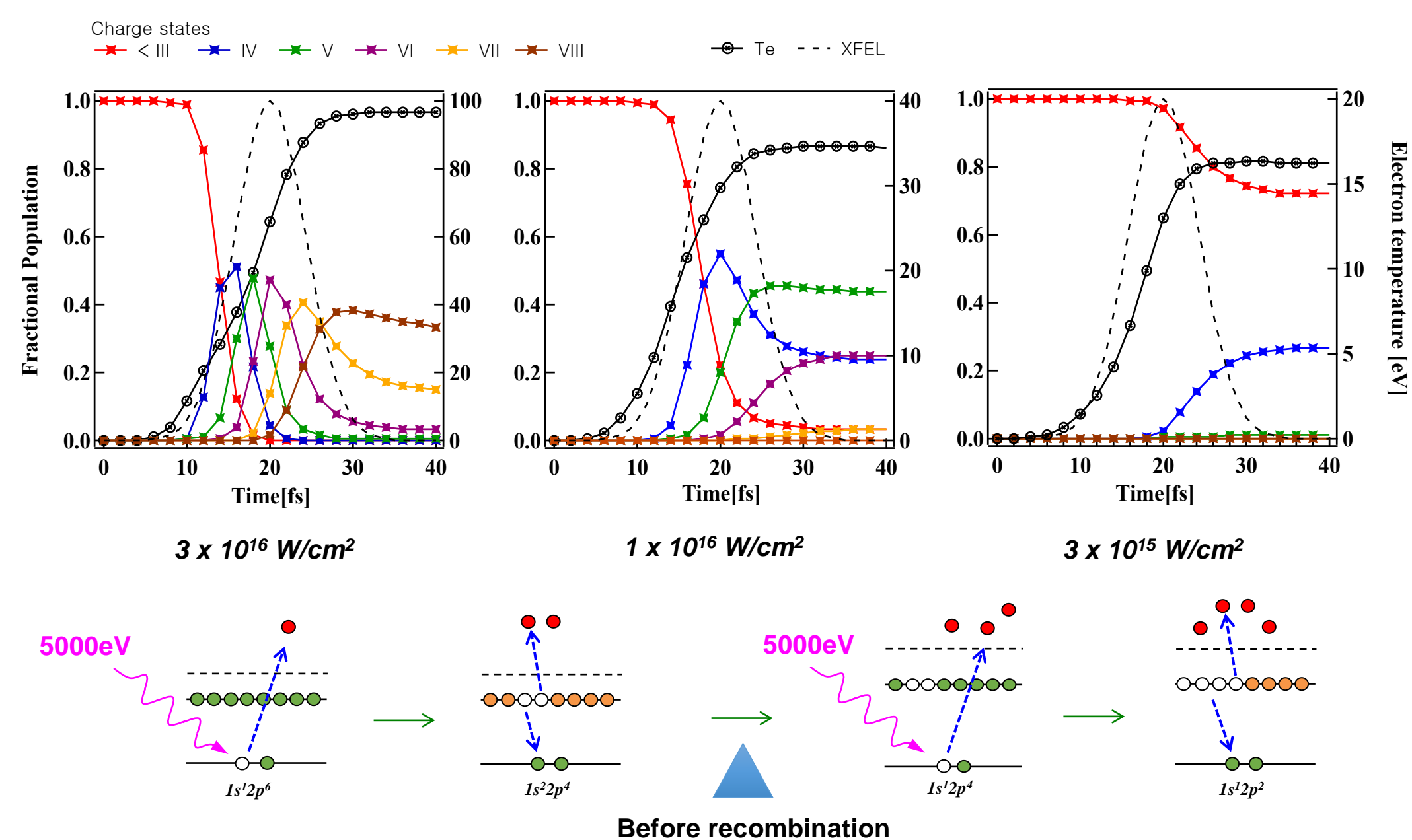


## Simulation results

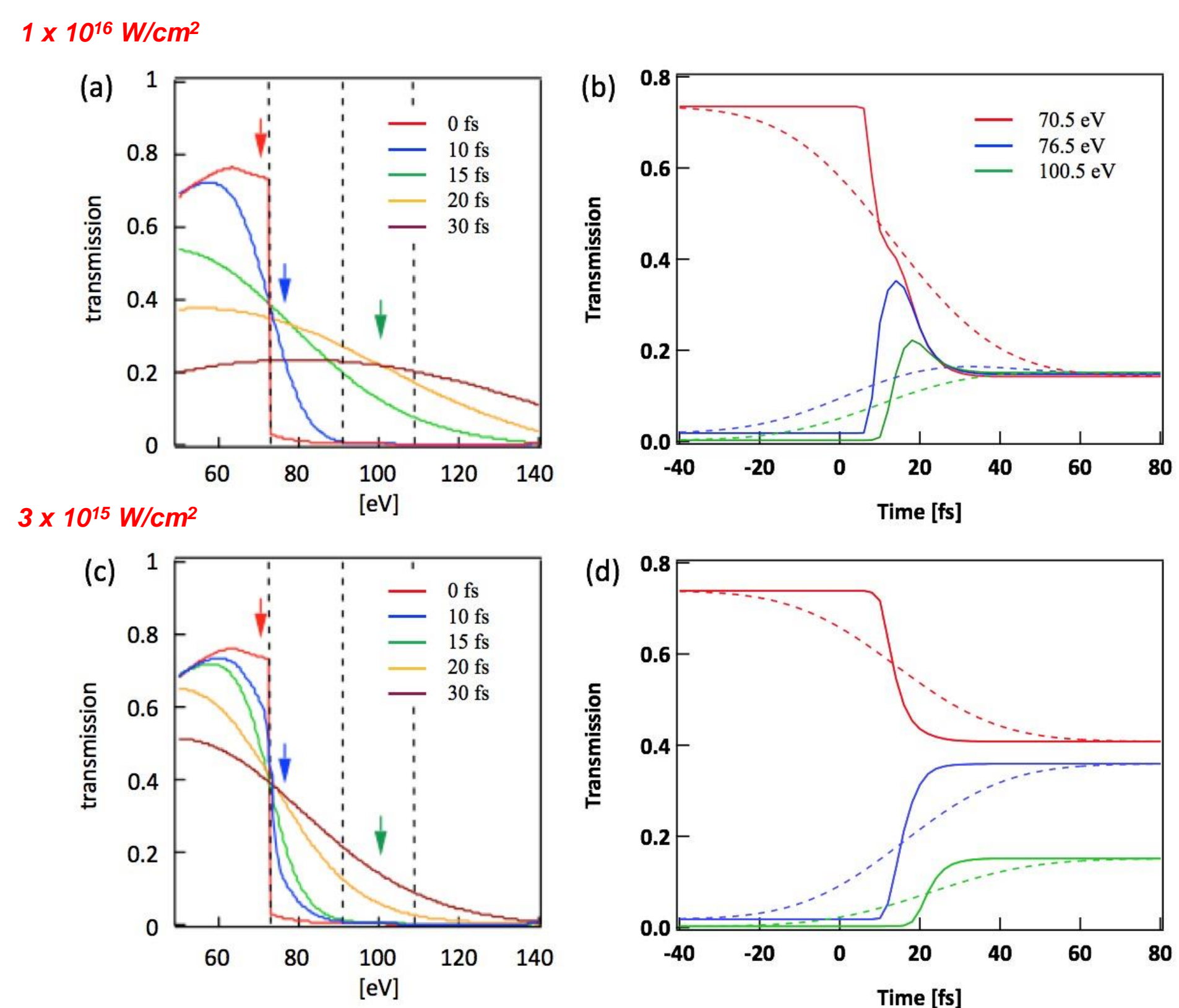
### Temporal evolution of Al charge state for various XFEL Intensity

- XFEL pulse, assumed as a Gaussian with 10 fs FWHM, is plotted as dash line.
- When the peak x-ray intensity is high (1x10<sup>16</sup> W/cm<sup>2</sup>), very high charge states, such as N- or B-like Al, could be developed with an electron temperature ~ 100 eV.
- With a relatively low intensity (3x10<sup>15</sup> W/cm<sup>2</sup>), ionization is limited to the charge state IV (F-like), and higher charge states are barely generated.

## Simulation results



### XUV transmissions near the cold L-edge of Al at various time delays



- (a) and (b) are for the peak XFEL intensity of 10<sup>15</sup>; (c) and (d) are for 10<sup>14</sup> W/cm<sup>2</sup>
- L-shell ionization energies for the neutral Al, F-, and O-like ions are shown as vertical dashed lines in (a) and (c).
- In (b) and (d), dashed lines shows the results of the convolution of simulation data with a 50 fs FWHM Gaussian distribution.
- When the x-ray intensity is low - early time of (a) or the entire (c), the edge broadening is the major effect.
- As x-ray intensity increases - later time of (a), neutral atoms are depleted, and absorption edge will be shifted to higher energy.

## Conclusion & Future works

- Simulations show a ultrafast time-resolved XUV absorption spectroscopy can follow up the ultrafast dynamics in the early stage of electronic transitions of a solid density Al warm dense matter created by an XFEL pulse.
- The SCFLY simulations also explain that for XFEL intensity of 1 - 10 x 10<sup>15</sup> W/cm<sup>2</sup>, aluminum will be heated to temperatures of a few tens eV and that the absorption around L-edge change with a time scale of 10 femtoseconds.
- It will be possible to figure out the electron-electron equilibration time in warm dense matter by using laser-based HHG with XFEL technology.