Numerical investigation of the dense photoionized aluminum plasma

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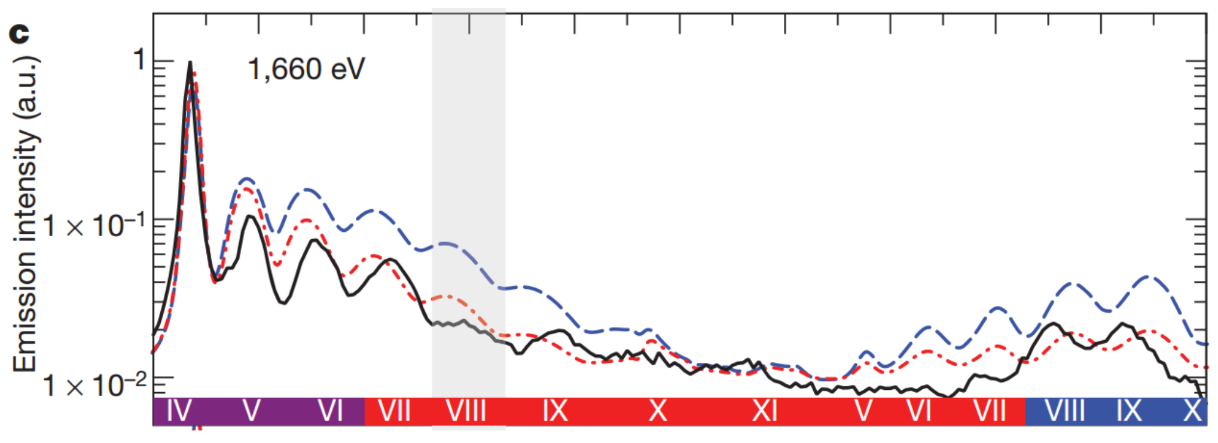
Problem overview

- The Linac Coherent Light Source (LCLS) was used to study solid-state aluminum plasma exposed to X-ray radiation with photon energies in the region of 1500– 1900 eV [1,2].
- The obtained emission spectra, containing the lines of transitions to the K shells for ions with a different charge, provide information on the structure of energy levels in plasma at high density, as well as on the shifts of the photoionization thresholds, line broadening and on the main processes (radiative and collisional).



- Due to the high density, there is a competition between the process of collisional ionization, Auger decay, and photoionization of the K-electron.
- The action of the X-ray beam is very short - 80 fs. Therefore, it is required to take into account the nonstationarity when calculating charge state distribution.

- The problem, simplified in the formulation, with parameters close to the experiment, was considered at the 10th Non-LTE code comparison workshop [13]
- The temperature versus time was calculated using SCFLY [14], the density is constant 2.7 g/cm^3. X-ray beam parameters are shown in the table below:

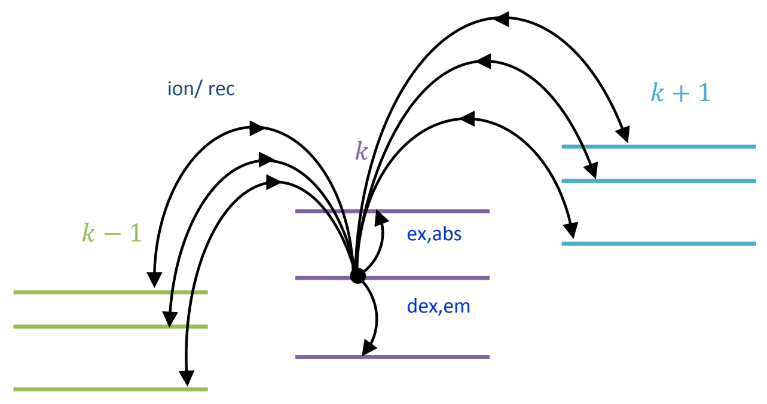
Erad (eV)	Bandwidth (eV)	Intensity (W/cm^2)	Field (J/cm^2/s/Hz/rad)	Duration (s)
1650	4.4	9.34×10^{16}	6.99	8×10^{-14}

THERMOS[3-8] code for Non-LTE plasma

Nonstationary rate equations

$$\frac{dx_{ks}}{dt} = \psi_{ks}(\vec{x}) - \varphi_{ks}\cdot x_{ks}$$

$$z_0 = \sum_{ks} k\cdot x_{ks},\ \sum_{ks} x_{ks} = 1,\ N_e = N_i\cdot z_0.$$



$$\psi_{ks}(\vec{x}) = \sum_{s'} \alpha^{ion/phi/ai}_{k-1s'\to ks}\cdot x_{k-1s'} + \sum_{s'} \alpha^{rec/phr/dr}_{k+1s'\to ks}\cdot x_{k+1s'} + \sum_{s'>s} \alpha^{dex/em}_{ks'\to ks}\cdot x_{ks'} + \sum_{s'<s} \alpha^{ex/abs}_{ks'\to ks}\cdot x_{ks'},$$

$$\varphi_{ks} = \sum_{s'} \alpha^{ion/phi/ai}_{ks\to k+1s'} + \sum_{s'} \alpha^{rec/phr/dr}_{ks\to k-1s'} + \sum_{s'<s} \alpha^{dex/em}_{ks\to ks'} + \sum_{s'>s} \alpha^{ex/abs}_{ks\to ks'}$$

- Equations were solved using a numerical scheme [9].
- Atomic data were obtained using the THERMOS code in the isolated ion approximation and corrected using the code FAC[10].

Ionization potential depression (IPD)

Stewart and Pyatt (SP) [11]: $\Delta I^{SP}(k) = \frac{3(k+1)}{2r_0}$, $r_0 = 1{,}388\left(\frac{A}{\rho}\right)^{1/3}$,

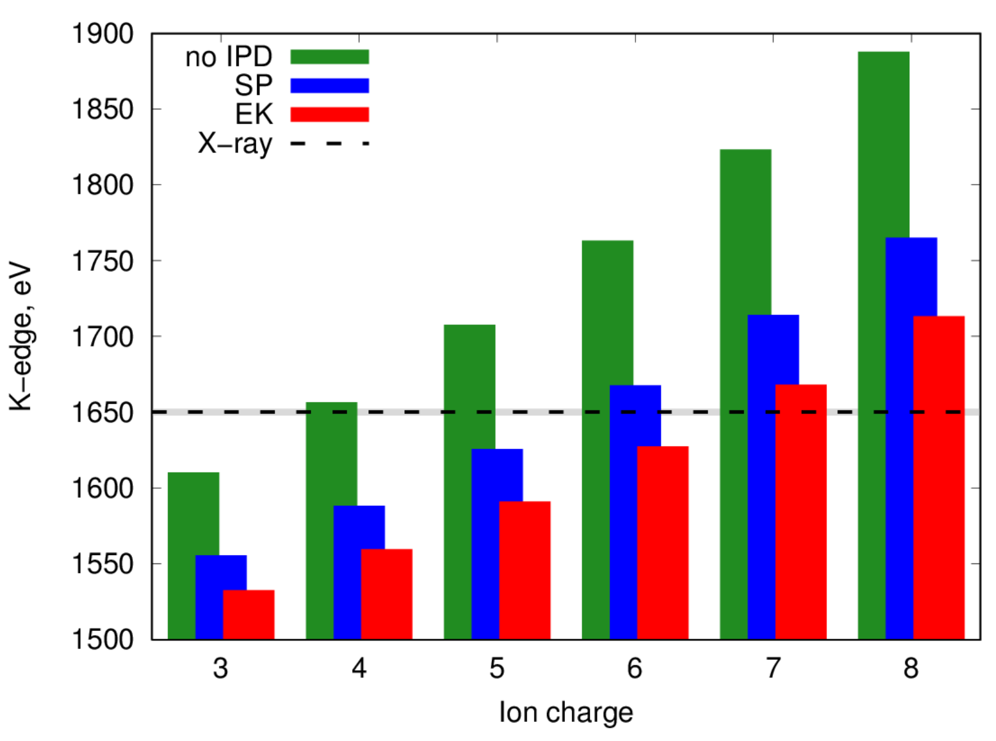
Ecker and Kröll (EK) [12]: $\Delta I^{EK}(k) = \frac{(k+1)}{r_{EK}}$, $r^3_{EK} = \frac{r^3_0}{1+Z_0}$.

Broadening of the photoionization cross-section threshold

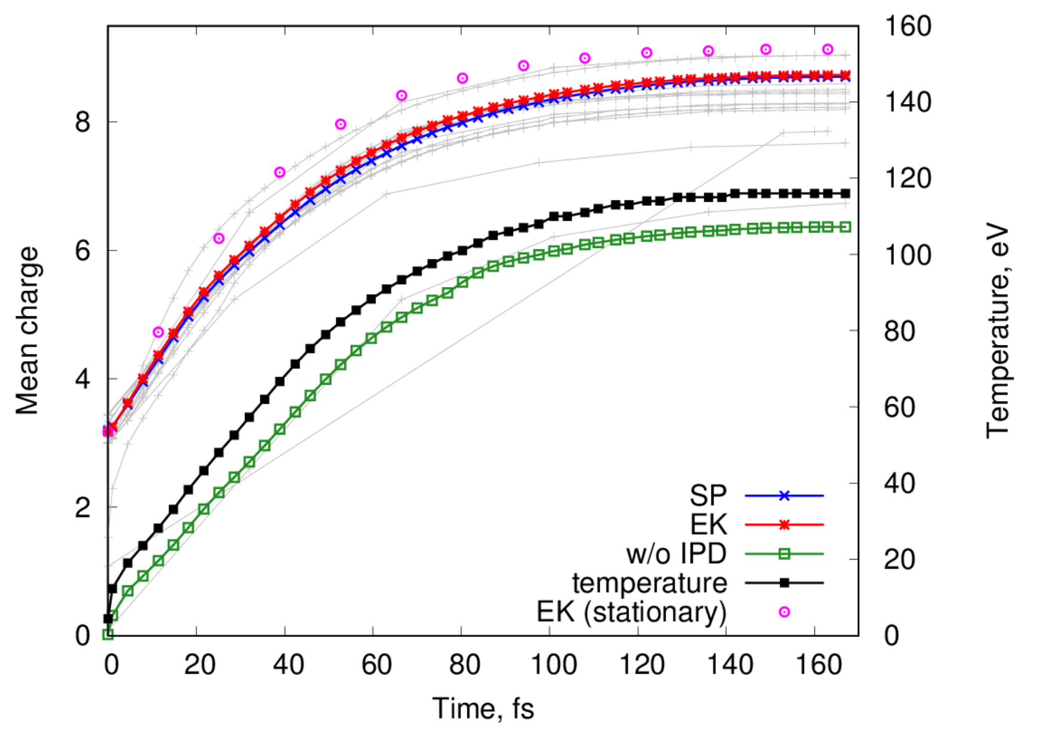
$$\tilde{\sigma}^{bf}_{nl}(\omega) = \sigma^{bf}_{nl}(\omega)\cdot\frac{1}{2}\left(1-\mathrm{erf}\left(\frac{\omega-\varepsilon^{IPD}_{nl}}{\Delta I^{IPD}}\right)\right),$$

$\varepsilon^{IPD}_{nl} = \varepsilon_{nl} - \Delta I^{IPD}$, ΔI^{IPD} - the shift of the photoionization threshold

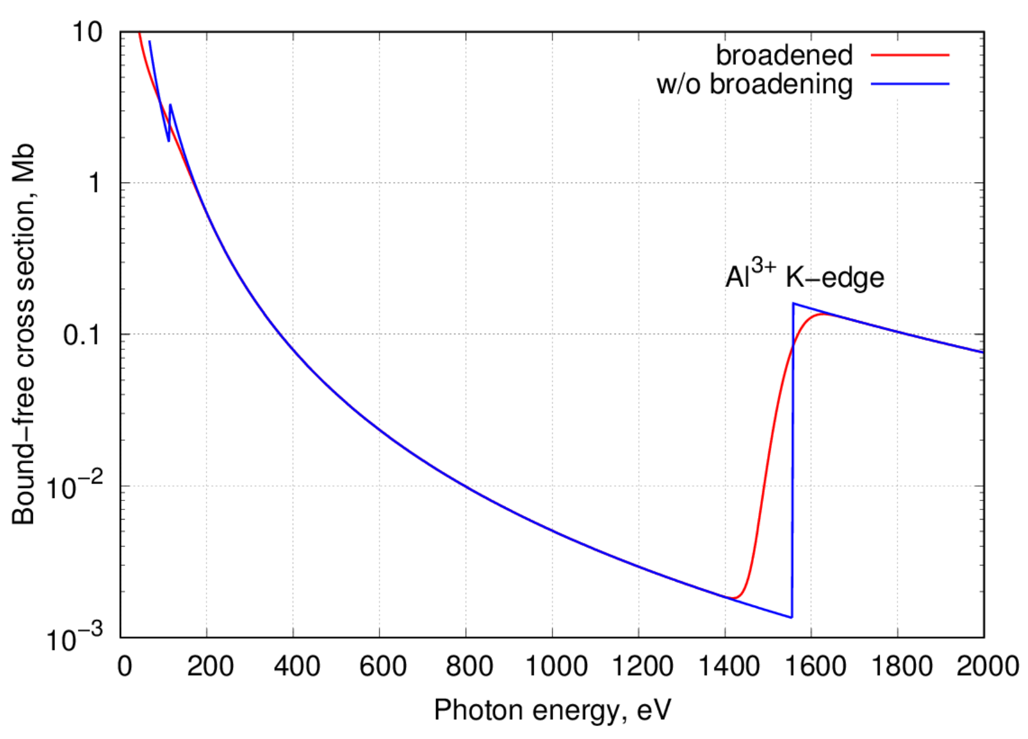
Simulation results



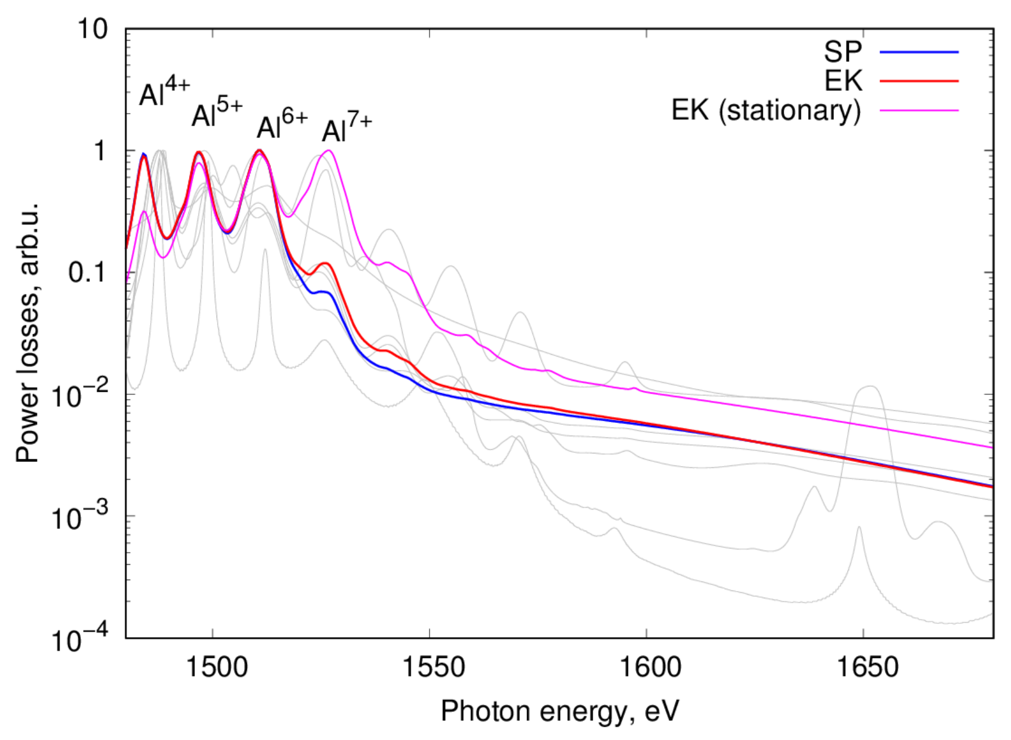
- The magnitude of the photoionization threshold shift determines which ions will have direct photoionization of the K-electron
- XFEL's monochromatic X-ray beams allow to experimentally determine this value and calibrate the theory



- The time dependence of the mean charge is in good agreement with calculations using other CR codes
- Due to the strong influence of collisional ionization, the calculation by the stationary CRE model gives close values of the mean charge, but the spectrum differs significantly
- The absence of density effects in calculation leads to an underestimation of the mean charge by about 3 times



- The procedure for effective broadening the photoionization thresholds allows us to take into account the influence of density effects and achieve a more correct form of the radiation spectrum



- The obtained spectra are in good agreement with the calculations of other scientific groups, and also have a qualitative similarity with the experimental one
- All the main processes determining the broadening of emission lines are taken into account
- The difference between the stationary and nonstationary variants is determined by the ratio between the rates of photoionization, Auger decay, and collisional ionization

Conclusions

✓Nonstationary solver for system of rate equations was implemented in the THERMOS Toolkit
✓It allows reproducing density effects and nonstationary effects
✓The THERMOS toolkit is suitable for simulation of XFEL experiments
✓The developed solver can be used in-line in 1D RGD codes

Acknowledgments

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References

[1] O. Ciricosta *et al.* Direct Measurements of the Ionization Potential Depression in a Dense Plasma, Phys. Rev. Lett. 109, 065002, 2012. DOI:10.1103/PhysRevLett.109.065002
[2] Vinko, S., Ciricosta, O., Cho, B. *et al.* Creation and diagnosis of a solid-density plasma with an X-ray free-electron laser. *Nature* 482, 59–62 (2012). https://doi.org/10.1038/nature10746
[3] THERMOS Toolkit http://keldysh.ru/thermos
[4] Nikiforov A.F., Novikov V.G., Uvarov V.B. Quantum-Statistical Models of Hot Dense Matter. Methods for Computation Opacity and Equation of State. Birkhauser, Basel, Switzerland, 2005. 428 pages. ISBN 987-3-7643-2183-8.
[5] KIAM_DB: atomic database for modeling of spectral properties of plasma 2016 /Novikov V.G. et al
[6] Nikiforov,A. F., Novikov V. G., Uvarov,V. B., VANT, 4(6), 16-26, 1979.
[7]Vichev, I.Y., Solomyannaya, A.D., Grushin, A.S., Kim, D.A. (2019). On certain aspects of the THERMOS toolkit for modeling experiments. *High Energy Density Physics*, 100713. https://doi.org/10.1016/J.HEDP.2019.100713
[8] V. G. Novikov, Average Atom Approximation in Non-LTE Level Kinetics, in: Y. Ralchenko (Ed.), Modern Methods in Collisional-Radiative Modeling of Plasmas, springer s Edition, Springer International Publishing, Switzerland, 2016, Ch. 5, pp. 105-126. doi:10.1007/978-3-319-27514-7_5.
[9] Belov A.A., Kalitkin N.N., Kuzmina L. V. Modeling of chemical kinetics in gases // Math. Model. Comput. Simulations. Pleiades Publishing, 2017. Vol. 9, № 1. P. 24–39.
[10] Gu M.F. Flexible Atomic Code (FAC) / M.F. Gu, E. Stambulchik
[11] Stewart J.C., Pyatt, Kedar D. J. Lowering of Ionization Potentials in Plasmas // Astrophys. J. 1966. Vol. 144. P. 1203.
[12] Ecker G., Kröll W. Lowering of the Ionization Energy for a Plasma in Thermodynamic Equilibrium // Phys. Fluids. American Institute of Physics, 1963. Vol. 6, № 1. P. 62.
[13] https://nlte.nist.gov/NLTE10/
[14] Orlando Ciricosta, Hyun-Kyung Chung, Richard W. Lee, Justin S. Wark, Simulations of neon irradiated by intense X-ray laser radiation, High Energy Density Physics, Volume 7, Issue 3, 2011, Pages 111-116, ISSN 1574-1818, https://doi.org/10.1016/j.hedp.2011.02.003.

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