Method for recovering soft X-ray emission spectra of plasmas from spectrograms recorded with a transmission diffraction grating

A A Kologrivov¹,², A A Rupasov¹ and G V Sklizkov¹

¹ Lebedev Physics Institute, Russian Academy of Sciences, 119991, Leninsky prosp. 53, Moscow, Russia
² E-mail: kologriv@sci.lebedev.ru

Abstract. An iterative method was developed for recovering soft X-ray emission spectra from spectrograms obtained using a transmission diffraction grating. The method was compared with another one that was previously used. In the case of a linear radiation detector, both these methods are almost equivalent. In the case of a nonlinear detector, the method used previously could not be used, whereas the new method provides high-quality recovery of X-ray spectra.

1. Introduction

Obtaining a real spectrum from spectrograms recorded using a transmission diffraction grating (TDG) is complicated by the partial overlap of different diffraction orders on a detector (for example, a CCD array or a film), which distorts the real shape of the spectrum. In the case of a discrete lines spectrum, this does not lead to any difficulties because the same spectral lines are strictly repeated in different diffraction orders (due to linear dispersion) and they can be easily identified. However, in the case of a continuous spectrum, the overlap of different diffraction orders in the spectrogram makes the determination of the correct shape of this spectrum a problem. An analytic solution to this problem has not been determined. Thus, we developed an iterative method for recovering spectra [1] using an algorithm of successive calculation corrections of the recorded diffraction pattern using a TDG.

To substantiate the efficiency of the developed algorithm, we performed test calculations, for example, in which an arbitrary spectrum (called the initial spectrum) was specified because the spectrum that is recovered is unknown in real experiments.

2. Iterative method of spectrum recovery

We solved a direct problem for the initial spectrum, namely, the grating response to this spectrum was calculated, i.e., we calculated the superposition of a certain number (5–7) of the most intense diffraction orders. Then, the initial spectrum was reconstructed using the iterative method beginning from the choice of the zero-order approximation. As a zero-order approximation, a spectrum from a quite broad set of functions can be used, e.g., the equilibrium emission spectrum of a plasma at some temperature. Then, the grating response to the chosen zero-order approximation spectrum was calculated. Then, the zero-order approximation spectrum was multiplied by the ratio of the grating response on the initial spectrum to the grating response on the zero-order approximation spectrum. The result was obtained in the first-order approximation. Each subsequent approximation was obtained...
from the previous one via the same rule. The process was finished when the difference between the
response on the \( n \)-order approximation spectrum and the response on the initial spectrum became
smaller than the specified value (usually \( \sim 2\% \)). This was achieved for most of the initial spectra
chosen for testing after 3–11 iteration steps.

The number of diffraction orders that should be taken into account in this algorithm depends on the
ratio of gap \( \delta \) (the transmission part of a structure period) to period \( d \). Expressions that determine the
inaccuracy caused by the neglect of high-order diffraction orders have been derived in ref. [1]. These
expressions show that consideration of the 5–7 diffraction orders provides a sufficient accuracy of
\( \sim 2\% \).

As an example, we demonstrate in Figure 1 the recovery of the emission spectrum of a plasma
containing 95\% free electrons with an electron temperature of \( T_e = 400 \) eV and 5\% of free electrons
with a temperature of \( T_e = 2 \) keV for a grating with a ratio of \( \delta/d = 1/2 \). In this example, the third
approximation already coincides with the specified spectrum with such a good accuracy that they are
indiscernible in the plot. The divergences of the iterative process for gratings with \( \delta/d = 1/2, 1/3 \) and
1/4 and for different zero-order approximations are also shown in Table 1.

![Figure 1](image)

**Figure 1.** Initial spectrum of a two-electron plasma (solid curve), the
superposition of the first, third and fifth diffraction orders (dashed curve),
zero-order approximation (spectrum \( T_e = 400 \) eV, dotted curve 0), first-order
approximation (dot-and-dash curve 1), and second-order approximation (dot-
and-dash curve 2) for a grating with \( \delta/d = 1/2 \).

The iterative calculations presented above lead to the following conclusions:

(i) Beginning from some approximation, the recovered spectrum no longer changes and virtually
coincides with the specified spectrum. The best results are obtained for a grating with \( \delta/d = 1/2 \), when
the minimal number of diffraction orders and iterations should be taken into account. For a grating
with \( \delta/d = 1/3 \), the required number of diffraction orders and iterations taken into account increases.
For a grating with \( \delta/d = 1/4 \), this tendency remains; however, it does not lead to a considerable
increase in the number of iterations.

(ii) The convergence rate and the spectrum recovery accuracy were virtually tested in our work,
which demonstrated the applicability of the developed algorithm for recovering the real spectrum from
the recorded spectrograms.

All the above considerations concern the linear radiation detectors, i.e., detectors for which the
output signal intensity is proportional to the radiation spectral intensity of a source and is independent
of the wavelength.
Table 1. Process convergence for a spectrum of two-temperature plasma (95% of electrons with a temperature of $T_e = 400$ eV and 5% of electrons with a temperature of $T_e = 2$ keV). $\delta/d$ is the grating gap/period ratio; $N$ is the successive approximation number; $\xi$ is the maximum deviation of the response on the spectrum recovered at the current iteration to the response on the real spectrum; and $\lambda_m$ is the wavelength at which this deviation is observed. As the zero-order approximation, the emission spectrum of an equilibrium plasma was used with the electron temperature indicated in the top line of the table.

| $\delta/d = 1/2$; $T_e = 400$ eV | $\delta/d = 1/2$; $T_e = 300$ eV | $\delta/d = 1/2$; $T_e = 600$ eV | $\delta/d = 1/3$; $T_e = 400$ eV | $\delta/d = 1/4$; $T_e = 400$ eV |
|------------------------------|------------------------------|------------------------------|------------------------------|------------------------------|
| $N$ | $\xi$ | $\lambda_m$, Å | $\xi$ | $\lambda_m$, Å | $\xi$ | $\lambda_m$, Å | $\xi$ | $\lambda_m$, Å | $\xi$ | $\lambda_m$, Å |
| 0 | 1.256 | 3 | -1.256 | 3 | -1.256 | 3 | -1.25599 | 3 |
| 1 | 0.177 | 11 | 0.181 | 11 | 0.157 | 10 | 0.337 | 8 | 0.71844 | 6.5 |
| 2 | 0.022 | 11 | 0.0228 | 11 | -0.0277 | 36 | 0.055 | 5.5 | 0.20833 | 6.5 |
| 3 | 0.0053 | 11 | 0.00538 | 11 | -0.00893 | 39 | -0.01582 | 22 | -0.08710 | 14 |
| 4 | 0.00324 | 11 | 0.00324 | 11 | 0.00319 | 11 | 0.00642 | 4.5 | -0.06001 | 14 |
| 5 | 0.00297 | 11 | 0.00297 | 11 | 0.00297 | 11 | 0.00525 | 4.5 | -0.03322 | 14 |
| 6 | 0.00294 | 11 | 0.00294 | 11 | 0.00294 | 11 | 0.00503 | 4.5 | -0.01636 | 14 |
| 7 | 0.00294 | 11 | 0.00294 | 11 | 0.00294 | 11 | 0.00499 | 4.5 | 0.01241 | 27 |
| 8 | 0.00294 | 11 | 0.00294 | 11 | 0.00294 | 11 | 0.00498 | 4.5 | 0.01008 | 4.5 |
| 9 | 0.00294 | 11 | 0.00294 | 11 | 0.00294 | 11 | 0.00498 | 4.5 | 0.01000 | 4.5 |
| 10 | 0.00294 | 11 | 0.00294 | 11 | 0.00294 | 11 | 0.00498 | 4.5 | 0.00998 | 4.5 |
| 11 | 0.00294 | 11 | 0.00294 | 11 | 0.00294 | 11 | 0.00498 | 4.5 | 0.00997 | 4.5 |
| 12 | 0.00294 | 11 | 0.00294 | 11 | 0.00294 | 11 | 0.00498 | 4.5 | 0.00997 | 4.5 |

3. Comparison with other iterative algorithms and conclusions

In ref. [2], another iterative algorithm was proposed in which, unlike our algorithm, the difference of responses was determined rather than their ratio by comparing the response of the recovered spectrum at the $n$-th iteration step with the response to the experimental spectrum. To determine the $(n+1)$ iteration spectrum, this difference was subtracted from the $n$-th iteration spectrum.

A comparison of the two algorithms showed that their results are approximately the same in the case of a linear detector (Figure 2). It is seen in Figure 2 that algorithm [2] requires a smaller number of iterations for spectrum recovering. Thus, our algorithm provides a result that coincides with the initial spectrum after the 11th iteration, whereas the calculations performed in accordance with the algorithm from ref. [2] lead to a similar result after the 6th iteration.

A completely different situation occurs in the case of a nonlinear detector, e.g., a film. In the real case, the exposition in each region of the film is determined by a sum of expositions from emission wavelengths that correspond to different diffraction orders. The film parameters (sensitivity and contrast) depend on the wavelength, whereas the film optical density, $D$, depends nonlinearly on the
light intensity, and $D$ is not equal to the sum of optical densities $D_n$ (where $D_n$ is the film optical density caused by the light exposition in the $n$-th diffraction order in the given film region).

![Intensity, a.u. vs. Wavelength, Å](image)

**Figure 2.** Example of spectrum recovery by the method proposed for a grating with $\delta/d = 1/4$ after 6 iterations (1) and after 11 iterations (2). Spectrum 2 coincides with the spectrum obtained by the method from ref. [2] after 6 iterations.

Nevertheless, if we take the film sensitivity and contrast that correspond to wavelengths in the first diffraction order, the final result does not considerably change. Indeed, the inverse problem is in fact the process of finding a spectrum that produces the required optical density, whereas the direct problem of determining the optical density caused by the given spectrum is solved exactly (accurately to neglected higher-diffraction orders). Such an approach always gives, at a certain iterative step, results in which the response on the recovered spectrum differs from that on the initial spectrum less than by the specified inaccuracy. This means that this iterative method is also applicable to the spectrum that is recorded in the case of a nonlinear detector.

As for the iterative method proposed in ref. [2], it turns out to be invalid for a nonlinear detector. An attempt to use this method leads either to negative intensity values in some regions of the spectrum after the 2nd or 3rd iteration (which is void of sense) or to the divergence of the process, i.e., the response at each next iteration differs from the initial spectrum more than at the previous iteration.

Thus, in the case of a linear radiation detector, both iterative methods can be used for spectrum recovering, whereas in the case of a nonlinear detector, only our developed method can be used.

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**References**

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