

# Signatures of $r$ -process elements in kilonova spectra

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**Abstract.** Binary neutron star (NS) mergers have been expected to synthesize  $r$ -process elements and cause electromagnetic radiation called kilonovae. Although  $r$ -process nucleosynthesis was confirmed by the observations of GW170817/AT2017gfo, individual elements have not been identified except for strontium. Toward identification of elements in kilonova spectra, we perform radiative transfer simulations in NS merger ejecta. We find that Sr II triplet lines appear in the spectrum, which is consistent with the absorption feature observed in GW170817/AT2017gfo. The synthetic spectrum also shows the strong Ca II triplet lines. Absence of the Ca II line features in GW170817/AT2017gfo implies that the Ca/Sr ratio is  $< 0.002$  in mass fraction, which is consistent with nucleosynthesis for electron fraction  $\geq 0.40$  and entropy per nucleon (in units of Boltzmann constant)  $\geq 25$ . Identification of absorption lines in near-infrared wavelengths which have not yet been decoded may lead to clarify the abundances synthesized in NS merger ejecta.

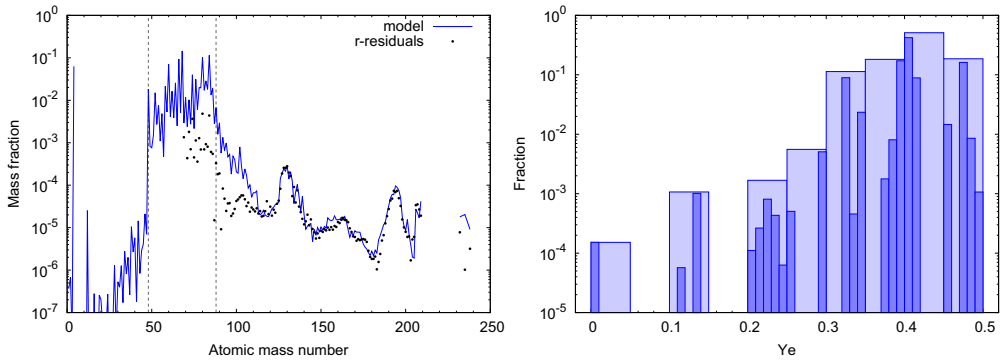
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## 1. Introduction

Binary neutron star (NS) mergers are promising sites for the rapid neutron capture nucleosynthesis ( $r$ -process, e.g., [Eichler et al. 1989](#)). A NS merger ejects neutron-rich material and heavy elements are synthesized in the ejecta. The subsequent radioactive decay of freshly synthesized nuclei powers electromagnetic emission, as called kilonova (e.g., [Li & Paczyński 1998](#)). A kilonova is expected to produce thermal emission mainly in ultraviolet (UV), optical and near-infrared (NIR) wavelengths.

In 2017, the first gravitational wave detection from a NS merger was successfully made (GW170817, [Abbott et al. 2017a](#)). Through the intensive follow-up observations, an associated electromagnetic counterpart was also identified (AT2017gfo, [Abbott et al. 2017b](#)). Observed properties of AT2017gfo in the UV, optical and NIR wavelengths are



**Figure 1.** Left: Final abundance for our model as a function of mass number. Black dots show the  $r$ -process residual pattern used for fitting (Prantzos et al. 2020). The residual abundances are scaled to match those for our model at  $A = 138$ . Vertical dashed lines indicate  $^{48}\text{Ca}$  and  $^{88}\text{Sr}$ . Right: Histograms of electron fraction  $Y_e$  for our model. Denser colors show the histograms with an original interval to construct the model ( $\Delta Y_e = 0.01$ ), while lighter colors show those with a grouped interval ( $\Delta Y_e = 0.05$ ) (Wanajo 2018).

broadly consistent with the theoretical expectation of kilonova, which has provided us with the evidence that NS mergers can be certainly the site of  $r$ -process nucleosynthesis.

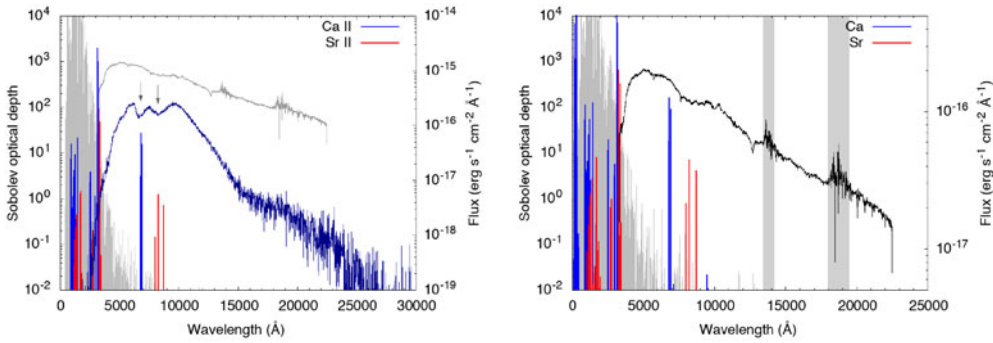
It is important to figure out the abundance patterns which NS mergers produce. This leads toward understanding of not only the origin of heavy elements but also the physical conditions for NS merger ejecta, i.e., their masses, velocities and electron fractions (the number of protons per nucleon,  $Y_e$ ). It is not yet clear, however, which elements are synthesized in GW170817, except for Sr (Watson et al. 2019). It is challenging to identify individual elements by using absorption features in the observed spectra since the absorption lines become broader and significantly overlapped in the high velocity ejecta. Toward extracting elemental information from kilonova spectra, we present the results of radiative transfer simulations in NS merger ejecta.

## 2. Radiative transfer simulations

We use a wavelength-dependent radiative transfer simulation code (Tanaka & Hotokezaka 2013, Tanaka et al. 2014, Kawaguchi et al. 2018). The photon transfer is calculated by the Monte Carlo method. For the ejecta density structure, we assume a single power law ( $\rho \propto r^{-3}$ ) for the velocity range of the ejecta  $v = 0.05\text{--}0.3 c$ . The total ejecta mass is set to be  $M_{\text{ej}} = 0.03 M_{\odot}$ . We calculate the Sobolev optical depth to evaluate the line strength of bound-bound transitions.

Atomic data are essentially important to evaluate the line strength. Since we focus on the imprints of elemental abundances in kilonova spectra, we construct the latest line list based on the Vienna Atomic Line Database (VALD, Piskunov et al. 1995). This database is suitable to identify lines because the transition wavelengths are calibrated with experiments and semi-empirical calculations.

For the abundance in the ejected matter from a NS merger, we use a model that fits the  $r$ -process residuals for  $A \geq 69$  and 3% of those for  $A \geq 100$ , where  $A$  is mass number. This model is constructed as an ensemble of the parameterized outflows with constant velocity, initial entropy, and initial  $Y_e$ , which fit the  $r$ -process residuals of the solar abundances (Prantzos et al. 2020), based on Wanajo 2018. We use the model dominated by relatively light elements (the left panel of Figure 1), since GW170817 was observed from the polar direction and the ejecta may be dominated by relatively high- $Y_e$  component (the right panel of Figure 1).



**Figure 2.** Left: Synthetic spectrum (blue curve) and line strength of each transition (vertical lines) at  $t = 1.5$  days. We plot the Sobolev optical depths in the ejecta at  $v = 0.2 c$ , which positions are blueshifted according to  $v = 0.2 c$ . Gray curve shows the spectrum of AT2017gfo at  $t = 1.5$  days, which is vertically shifted for comparison. Right: Comparison between the observed spectrum for AT2017gfo at  $t = 1.5$  days and the calculated Sobolev optical depths. The positions of lines are blueshifted according to  $v = 0.2 c$ . Gray shade shows the region of strong atmospheric absorption.

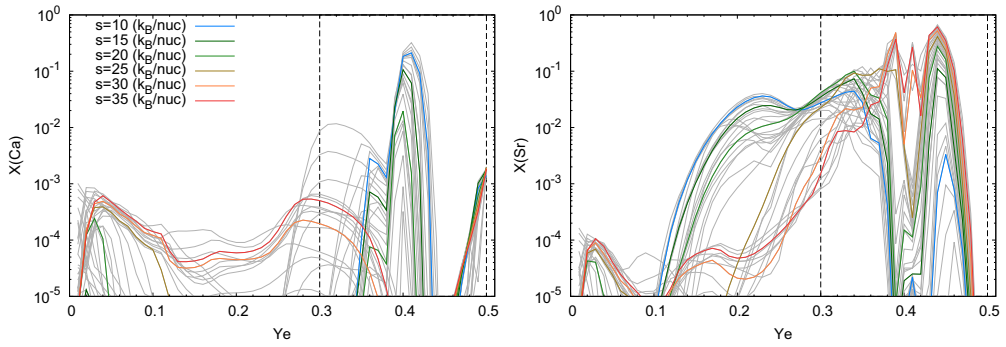
### 3. Results & Discussions

*Absorption features.* The left panel of Figure 2 shows our synthetic spectrum at  $t = 1.5$  days after the merger (blue curve). To show the contribution of different elements, we also plot the line strength in the ejecta at  $v = 0.2 c$ . The wavelengths of lines are blueshifted according to  $v = 0.2 c$ . We find that Sr II and Ca II produce absorption lines at  $\lambda \sim 8000 \text{ \AA}$  and  $\lambda \sim 6500 \text{ \AA}$ , respectively. It is natural that not only Sr II but also Ca II triplet lines become strong, because these elements have similar atomic structures. Both elements belong to the group 2 in the periodic table and have only one electron in the outermost shell when they are singly ionized. The electron occupies the *s* shell in the ground state and has a relatively small number of excited levels. Thus, the transition probability of each bound-bound transition tends to be high.

*Implications for AT2017gfo.* The right panel of Figure 2 shows comparison between the spectrum of AT2017gfo at  $t = 1.5$  days (Pian et al. 2017) and our results of the line strength. The wavelengths of the transitions are blueshifted according to  $v = 0.2 c$ . With this velocity, the wavelengths of the Sr II triplet (red) lines are consistent with the observed broad absorption feature. Although our synthetic spectrum suggests that Ca II can also exhibit strong absorption lines, the spectrum of AT2017gfo does not show such a feature at  $\lambda \sim 6800 \text{ \AA}$ , an expected wavelength of the Ca II triplet with  $v = 0.2 c$ . This implies that the abundance of Ca of AT2017gfo is smaller than that in our model. By varying the mass fraction of Ca, we find that the ratio  $X(\text{Ca})/X(\text{Sr}) < 0.002$  is required to reconcile our model with the case for AT2017gfo.

To infer the relevant physical properties from this constraint, we show the mass fractions of Ca and Sr as a function of  $Y_e$  for the results of nucleosynthesis calculations with different velocities and entropies in Figure 3. We here focus on the range of  $Y_e = 0.30\text{--}0.50$  as a relevant condition in our abundance model and the velocity of only  $v = 0.2 c$  which is consistent with the blueshift of the Sr II triplet in AT2017gfo. For these conditions, the condition of  $X(\text{Ca})/X(\text{Sr}) < 0.002$  can be achieved only with the relatively high entropies of  $s \geq 25 k_B/\text{nuc}$ . This implies that the blue component of AT2017gfo, which produces the Sr absorption line, comes from relatively high entropy ejecta.

Our results imply that the Ca triplet line can be observed in future NS merger events. It is also interesting to note that the isotope of calcium here is  $^{48}\text{Ca}$  whose origin is



**Figure 3.** Mass fractions of Ca (left) and Sr (right) as a function of  $Y_e$  for the results of nucleosynthesis calculations with the various sets of velocity and entropy (gray lines). Colored lines show the results with  $v = 0.2 c$  and the six different entropies in the legend. The Ca abundance is dominated by  $^{48}\text{Ca}$  except for  $Y_e \gtrsim 0.45$ .

unknown. If the absorption line caused by the Ca II triplet appears in future kilonova spectra, we will be able to confirm the production of  $^{48}\text{Ca}$  by NS mergers.

*Future work & prospects.* Our results suggest that we can directly obtain the evidences for synthesized each heavy element in the NS merger ejecta from observed spectra. Since the observed spectra of AT2017gfo have absorption features which have not yet been decoded, we still need to reveal them to clarify the abundances synthesized in the ejecta of GW170817.

While the observed spectra show absorption features in the NIR region, spectroscopically accurate atomic data needed to extract elemental information is currently limited especially for heavy elements in the NIR wavelengths. Thus, we have focused only on the spectral features made by some elements with available accurate data. Under such situation, atomic data constructed from theoretical calculations are often used for theoretical calculations of kilonova light curves (e.g., Tanaka *et al.* 2020). On the other hand, although such atomic data are useful in terms of data completeness, we cannot directly use the theoretical line list for element identification because the theoretical data are not necessarily accurate in terms of transition wavelengths. A hybrid line list which combines advantages of both line lists constructed from experimental database and theoretical calculations may lead to reasonable modeling of kilonova spectra to decode the entire spectral signatures.

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