[Co III] versus Na I D in Type Ia supernova spectra

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Accepted 2014 January 21. Received 2014 January 20; in original form 2013 October 29

ABSTRACT
The high metal content and fast expansion of supernova (SN) Ia ejecta lead to considerable line overlap in their optical spectra. Uncertainties in composition and ionization further complicate the process of line identification. In this paper, we focus on the 5900 Å emission feature seen in SN Ia spectra after bolometric maximum, a line which in the last two decades has been associated with [Co III] 5888 Å or Na I D. Using non-LTE time-dependent radiative-transfer calculations based on Chandrasekhar-mass delayed-detonation models, we find that Na I D line emission is extremely weak at all post-maximum epochs. Instead, we predict the presence of [Co III] 5888 Å after maximum in all our SN Ia models, which cover a range from 0.12 to 0.87 M⊙ of 56Ni. We also find that the [Co III] 5888 Å forbidden line is present within days of bolometric maximum, and strengthens steadily for weeks thereafter. Both predictions are confirmed by observations. Rather than trivial taxonomy, these findings confirm that it is necessary to include forbidden-line transitions in radiative-transfer simulations of SNe Ia, both to obtain the correct ejecta cooling rate and to match observed optical spectra.

Key words: radiative transfer – supernovae: general – supernovae: individual: 2005cf – white dwarfs.

1 INTRODUCTION
Radiative-transfer modelling of supernova (SN) Ia is a challenging enterprise (Eastman & Pinto 1993; Hoffman 1995; Baron et al. 1996; Pinto & Eastman 2000a,b; Höflich 2003; Kasen, Thomas & Nugent 2006; Jack, Hauschildt & Baron 2011; Dessart et al. 2013b, hereafter D13). For a start, the initial ejecta conditions for such simulations are uncertain. The possibility of both single- and double-degenerate progenitor systems suggests that the ejecta mass likely varies amongst SN Ia ejecta (e.g. Pinto & Eastman 2000a; Sim et al. 2010; van Kerkwijk, Chang & Justham 2010). The ejecta composition that results from the combustion of a C/O white dwarf is not known with confidence because the explosion scenario, besides being non-unique, involves hard-to-model combustion physics (Hillebrandt & Niemeyer 2000). As a result, for each scenario, simulations of the explosion, whether 1-D or multi-D, are parametrized rather than modelled consistently from first principles (Khokhlov 1991; Gamezo, Khokhlov & Oran 2005; Röpke & Hillebrandt 2005). The progenitor is likely to depart from a simple hydrostatic configuration for many possible reasons including fast rotation (Yoon & Langer 2004), the conditions produced by the smoldering phase and ignition (see e.g. Woosley, Wunsch & Kuhlen 2004), or from the complex dynamical evolution in a merger event (Pakmor et al. 2011, 2012).

Even if the ejecta properties were accurately known, the modelling of the radiation would remain challenging because of the prevalence of line opacity, the strong influence of scattering resulting from the very low gas densities in the fast expanding low mass ejecta, the importance of non-LTE and time-dependent effects, and non-thermal processes. Perhaps even more important are the numerous processes that take place between the various constituents of the gas (electrons and ions), involving thousands of atomic levels, and which control its thermodynamic state. Historically, this complexity has generally been interpreted in terms of an ‘opacity’ problem (see e.g. Hoflich, Mueller & Khokhlov 1993; Pinto & Eastman 2000b; Kasen et al. 2008). In D13, we demonstrate that the temperature and ionization distribution, which are difficult to determine accurately, are also important (not surprisingly) because the thermodynamic state of the gas determines which ions provide the opacity. We found, for example, that forbidden lines are crucial, as early as bolometric maximum, in controlling the cooling of the ejecta. Paradoxically, these lines have low oscillator strengths, and thus tend to be ignored in simulations prior to ≲100 d after explosion. Finally, inaccuracies in the atomic data, or the lack of atomic data altogether, introduce a major source of uncertainty in any radiative transfer modelling of SNe Ia.

A central problem with SNe in general is that lines are strongly Doppler broadened by the fast expansion of the ejecta. The large

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metal mass fraction in SNe Ia leads to the presence of forests of lines which overlap, typically preventing the identification of a ‘clean’ line anywhere in their spectra. The emerging radiation is in addition strongly influenced by a few strong lines, such as Si II 6355 Å or the Ca ii triplet, giving the wrong impression that the spectrum is analogous to a blackbody influenced by a few spectral features of large optical depth. This situation is particularly problematic when SNe Ia evolve past maximum because at such times, the optical depth clearly drops, the ejecta turns nebular, but strong lines are still present. There are no regions with negligible flux, even though the continuum optical depth is well below unity even at bolometric maximum (Hoeflich et al. 1993; Pinto & Eastman 2000b; Hillier, Dessart & Li 2013).

After bolometric maximum, the peaks and valleys of SN Ia spectra are a complex blend of numerous lines, some thick, others thin, each interacting with hundreds of other lines either locally (within a Sobolev length) or non-locally (because redshifted into resonance with a redder line). This conspires to produce confusion about spectrum formation in SNe Ia. The concept of a ‘photosphere’ is routinely used but the notion of a sharp boundary from where radiation would escape does not hold for SNe Ia. Branch et al. (2008) propose that most/all lines at nebular times are permitted (generally resonance) transitions, while numerous papers emphasize the near exclusive presence of forbidden-line transitions (Kuchner et al. 1994; Mazzali et al. 2008).

To give additional evidence for the importance of forbidden lines in SNe Ia (D13), we focus here on the 5900 Å feature observed in post-maximum SN Ia spectra. In recent years, this feature has been associated with Na I D, although this association remains suspicious and puzzling. Models sometimes provide a very good fit (Mazzali et al. 2008, fig. 3), a poor fit (Branch et al. 2008), or predict no feature at that location (Kasen, Röpke & Woosley 2009; Blondin et al. 2011; Tanaka et al. 2011). In the next section, we give an historical perspective of earlier work that modelled or discussed the spectral feature at 5900 Å. We then present results from our grid of delayed-detonation and pulsational-delayed-detonation models covering a range of 56Ni mass and show that this feature can be explained as [Co III] 5888 Å emission, across the range from subluminous to standard SNe Ia (Section 3). In other words, we find that such ejecta models naturally produce an emission feature at 5900 Å, and that this emission in our models is systematically associated with [Co III] 5888 Å. Our conclusions and a discussion of future work are presented in Section 4.

Far from being a banal characteristic of SN Ia spectra, the observation of the [Co III] 5888 Å line indicates that forbidden line transitions have to be incorporated in any SN Ia model at and beyond bolometric maximum, not just to reproduce observations, but also to compute correctly the cooling of SN Ia ejecta.

2 PREVIOUS WORKS

The spectral feature at 5900 Å in SNe Ia has been discussed repeatedly in the last two decades. We can separate the studies focusing on the ‘photospheric’ phase (epochs until soon after bolometric maximum) and those devoted to ‘advanced’ nebular phase (beyond 100 d after explosion when the SN exhibits an apparently pure-emission spectrum).

Axelrod (1980) is probably the first to study nebular-phase spectra of SNe Ia, and he associates unambiguously the 5900 Å feature with the forbidden transition of Co ii at 5888 Å. Later, Eastman & Pinto (1993) present numerical developments incorporated into the code EDDINGTON, and apply their technique to spectrum formation in a SN Ia ejecta at 250 d after explosion. They propose [Co iii] as the origin of the 5900 Å feature (see their fig. 5). Kuchner et al. (1994) use the simultaneous presence of [Co III] 5888 Å and [Fe II] 4658 Å (strictly speaking, the 4500–5000 Å region contains lines from both Fe ii and Fe iii) in SN Ia spectra to confirm the radioactive decay of 56Ni at the origin of the SN Ia luminosity. Indeed, they find the flux ratio of these two lines (ignoring line overlap and some complications of the radiative transfer) can be explained from the decay of 56Co to 56Fe. They discard the possible association of the 5900 Å feature with Na. Mazzali et al. (1997) study SN 1991bg at both early times and late times. At nebular times, they propose that the 5900 Å feature is primarily associated with [Co iii], and show how this Co forbidden transition may be used to set constraints on the original 56Ni mass. Their nebular model reproduces the 5900 Å feature, in both strength and width (see their fig. 14), supporting the same assessment made by Kuchner et al. (1994).

Disparate interpretations seem to start with the work of Lentz et al. (2001) who fail to reproduce the 5900 Å region of SN 1994D at early post-peak epochs, despite strong modulations of the adopted Na abundances in their ejecta model. They suggest that the explosion model employed is probably inadequate, but it also seems that they do not include forbidden-line transitions in the radiative-transfer modelling. Branch et al. (2008) use SYNOW to identify the lines present in SNe Ia after bolometric maximum and conclude that most lines are permitted. They also argue for a Na I D association with the 5900 Å feature (the broad absorption they predict is, however, associated with a broad line emission that is unseen), and while they mention the [Co iii] possibility they do not retain it. Mazzali et al. (2008) present an analysis of SN 2004eo spectra. They associate the 5900 Å emission feature at 250 d after explosion with Na i D. At earlier times, they suggest the 5900 Å feature is due to Si ii – it seems that no [Co iii] line is included in their modelling. Along the same reasoning, Tanaka et al. (2011) tie the 5900 Å feature to Na i D in SN 2003du, although the feature is not fitted by their model.

Maurer et al. (2011) perform detailed non-LTE steady-state radiative-transfer calculations at nebular times and explicitly discuss [Co iii] line emission. Although the strength of [Fe II] and [Co III] lines varies between codes, sometimes significantly, [Co iii] remains the most plausible explanation for the 5900 Å line.

It thus seems that from being secure in the 90s, the association of the 5900 Å feature with the [Co III] 5888 Å line is no longer retained, even though the Na i D association is rarely matched satisfactory by

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Table 1. Summary of nucleosynthetic yields for the Chandrasekhar-mass delayed-detonation models used in this work. Numbers in parenthesis correspond to powers of 10.

| Model | M(56Ni) [M⊙] | M(Ni) [M⊙] | M(Fe) [M⊙] | M(Si) [M⊙] | M(Na) [M⊙] |
|-------|--------------|------------|------------|------------|------------|
| DDC0  | 0.869        | 0.872      | 0.102      | 0.160      | 6.22(−6)   |
| DDC6  | 0.722        | 0.718      | 0.116      | 0.216      | 1.02(−5)   |
| DDC10 | 0.623        | 0.622      | 0.115      | 0.257      | 1.26(−5)   |
| DDC15 | 0.511        | 0.516      | 0.114      | 0.306      | 1.70(−5)   |
| DDC17 | 0.412        | 0.421      | 0.112      | 0.353      | 2.53(−5)   |
| DDC20 | 0.300        | 0.315      | 0.110      | 0.426      | 3.53(−5)   |
| DDC22 | 0.211        | 0.231      | 0.107      | 0.483      | 6.30(−5)   |
| DDC25 | 0.119        | 0.142      | 9.80(−2)   | 0.485      | 1.51(−4)   |
| PDDEL3| 0.685        | 0.680      | 0.107      | 0.218      | 1.57(−5)   |
Figure 1. Montage of spectra comparing our grid of delayed-detonation models (red) with observations (black) at $\sim 40$ d after $B$-band maximum (see left label). This plot is a counterpart of fig. 5 of Blondin et al. (2013) which makes a similar comparison near bolometric maximum (we have replaced SN 1992A by SN 2004eo since the former does not have data at this post-explosion epoch). For each pair, we give the $B$-band magnitude offset at the corresponding time (blue label on the right). The filled area coloured in red corresponds to the synthetic flux associated with the [Co III] 5888 Å forbidden-line transition.
SN Ia radiative-transfer models. Following upon our recent study of SN Ia physics and spectrum formation (D13), we study the origin of the 5900 Å feature in post-maximum SN Ia spectra using CMFGEN and our most complete model atom (see D13 for details). For this purpose, we use the same delayed detonation models with which we obtain good agreement to maximum-light spectra of SNe Ia (Blondin et al. 2013). We also include one pulsational-delayed-detonation model from Dessart et al. (2013a), model PDDEL3, since it yields a satisfactory match to the SN Ia 2005cf evolution from about −10 to +80 d. In numerous ways, the match is superior to that obtained with model DDC10, for reasons that we discuss in Dessart et al. (2013a).

3 RESULTS FROM DELAYED-DETONATION MODELS

In this paper, we use a sample of simulations from Blondin et al. (2013), D13, and Dessart et al. (2013a). All are delayed detonations (DDC sequence), but some explode following a pulsation (PDDEL sequence; see Dessart et al. 2013a for details). We summarize the key nucleosynthetic yields for these models in Table 1.

For the discussion of the paper, it suffices to say that these models cover a range of 56Ni mass, from 0.12 to 0.87 M⊙, and provide a satisfactory match to a wealth of SNe Ia at maximum light (Blondin et al. 2013). A fundamental property of all our delayed detonation models is that the sodium mass fraction below 15 000 km s⁻¹ is of the order of 10⁻⁵. The total sodium mass in our models is typically of the order of 10⁻⁴ M⊙.

In D13, we described how one must exert extreme care to account for a number of critical non-LTE processes in order to follow the SN Ia evolution from maximum light to the nebular phase. This not only requires a detailed account for opacity sources, especially associated with metals, but also for critical coolants which act as primary ingredients for setting the temperature and ionization state of the gas. So, each model we present here was evolved from 1 d to 100 d after explosion with all the key processes we found to be important (D13).

It would be presumptuous to pretend that with eight delayed-detonation models, we could reproduce all SNe Ia that exist. Instead, our strategy is to identify key signatures that characterize and distinguish SNe Ia, and test whether such delayed-detonation models predict those key signatures, without any tinkering of our hydrodynamical models (on composition, density profile, total mass, etc.). This strategy is sound because SNe Ia constitute a highly homogeneous class of events once we exclude the less frequent 91bg-like and 91T-like events. If a given explosion model has any validity, it should reproduce at least a subset of SNe Ia. We suspect this degeneracy calls for a similar degeneracy in SN Ia ejecta, and our simulations of delayed detonations confirm this.

In Fig. 1, we present a counterpart of the montage of B-band maximum spectra presented in Blondin et al. (2013), but this time for an epoch of ~40 d after B-band maximum. At this time, SNe Ia exhibit a very different spectral morphology, with a reduced flux in the blue and a dominance of metal lines, in particular from iron around 5000 Å. In this montage, we can clearly see that a broad feature is present around 5900 Å in all SNe Ia selected (which are quite typical of the SN Ia population as a whole), and therefore, that this feature is present whether we consider a luminous SN Ia like 1999ee or a sub-luminous SN Ia like 1999by.

Interestingly, all our delayed-detonation models predict a feature near 5900 Å. At 40 d past B-band maximum, the spectrum forms in the inner ejecta at velocities ≲10 000 km s⁻¹, although some photons will still experience scattering and absorption at larger velocities if they overlap with strong lines (primarily from intermediate-mass elements) or if they lie in the UV range. In the inner ejecta, our models have a composition dominated by cobalt and iron. As mentioned above, delayed detonation models leave no trace of sodium shown in Table 1 with the observed feature, we recompute the synthetic spectra but set the oscillator strength of that forbidden-line transition to zero. The resulting synthetic spectra are indistinguishable, apart from a strong difference in the 5900 Å region. The associated flux difference is shown as a filled area coloured in red.

After the detailed discussion presented in D13, it is not surprising that this feature is indeed primarily due to [Co ii] 5888 Å. And this explanation is more sensible from the point of view of nucleosynthesis since the sodium mass fraction in the inner ejecta is vanishingly small in all delayed-detonation models.

A further confirmation of this association is that the observed strength of the 5900 Å feature typically increases after bolometric maximum. In the context of [Co ii] emission, this also makes sense since the strength of forbidden lines relative to other lines should increase as the ejecta density drops. We show in Fig. 2 a montage of spectra for the evolution of SN 2005cf and model PDDEL3 (Dessart et al. 2013a) from bolometric maximum (i.e. +0 d) until +80 d (we note that model DDC10 studied in detail in D13 does a somewhat better job in the B-band region, but model PDDEL3 is more compatible with the narrow line profiles of SN 2005cf; both models are equally suitable for the present discussion). As in Fig. 1, we show the flux associated with the [Co ii] 5888 Å line as a filled red area. It is clearly evident that early after bolometric maximum, flux from that forbidden line contributes to the emergent radiation, and that this flux contribution increases with time, as observed. We note that at bolometric maximum, [Co ii] 5888 Å line emission is already a strong coolant of the Co-rich layers; [Co iii] 5889 Å line photons are not seen earlier on because these regions are located below the last scattering/absorbing layer.

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1 Part of the confusion has undoubtedly arisen because forbidden line emission is generally associated with low density, and thus the detection of a feature at 5900 Å not long after maximum would seem to preclude its identification with a forbidden line. A key distinction, however, is that Co is not an impurity species, and thus it is much more likely to be seen even though ejecta densities exceed the critical density.

| λ [Å] | Transition | f | A [s⁻¹] |
|-------|------------|---|--------|
| [Co ii] | 5627.104 | 3d¹ ⁴F [9/2] - 3d² ⁴G [7/2] | 5.323 (−11) | 0.0140 |
| [Co ii] | 5888.482 | 3d¹ ⁴F [9/2] - 3d² ⁴G [7/2] | 2.081 (−9) | 0.4001 |
| [Co ii] | 5906.783 | 3d¹ ⁴F [7/2] - 3d² ⁴G [7/2] | 7.850 (−10) | 0.1500 |
| [Co ii] | 6195.455 | 3d¹ ⁴F [7/2] - 3d² ⁴G [7/2] | 8.636 (−10) | 0.1200 |
| [Co ii] | 6576.309 | 3d¹ ⁴F [9/2] - 3d² ⁴G [5/2] | 1.868 (−10) | 0.0480 |
Figure 2. Montage of spectra comparing the observations of SN 2005cf (black) with model PDDEL3 (red; Dessart et al. 2013a). The filled area coloured in red corresponds to the synthetic flux associated with the [Co III] 5888 Å forbidden-line transition. Times are with respect to B-band maximum. Each model spectrum is reddened, redshifted, and scaled to match the inferred distance to SN 2005cf. A vertical scaling is used at each epoch for better visibility. However, the label on the right gives the B-band magnitude offset between model and observation at the corresponding epoch.
There are other [Co\textsc{iii}] lines in the 6000 Å region (Table 2). Of all these, the transition at 5888 Å is the strongest. The transition at 5906 Å is expected to be weaker and it also overlaps with the 5888 Å transition. The transition at 6195 Å should be about 1/3 of the strength of 5888 Å but the model predicts essentially no flux in this line. We find that the 6195 Å suffers absorption by overlapping lines, in particular from the \textsc{Si ii} doublet at 6355 Å, which is strong at those epochs. Numerous other lines are present in this spectral region, while fewer reside in the 5900 Å region, allowing the [Co\textsc{iii}] 5888 Å to escape. We also find that these low-lying states are in LTE with the ground state (they have the same departure coefficients), although we obtain strong depopulation (and strong departure from LTE) of the ground state of Co\textsc{iii} through non-thermal ionization and excitation (this departure is also epoch dependent). Scattering is thus expected to influence little the formation of these forbidden-line transitions.

We also see that in our simulations, the delayed detonation models systematically show a range of optical colours at +40 d, while observations look more similar at this time (Fig. 1). This is particularly visible for the low-luminosity SN Ia 1999by, which shows a stronger [Co\textsc{iii}] 5888 Å line and relatively less flux in the red than in our model DDC25. This range in colours in our models reflects the trend in ionization level at the corresponding epoch, as evidenced by the ionization state of Co in the inner ejecta where the spectrum forms (Fig. 3). This could arise from problems with the atomic physics, or from issues with the structure computed for the assumed progenitor model. Another possible explanation may be that, while the \textsuperscript{56}Ni mass is accurate in each model/observation pair (tightly constrained by the peak luminosity), the ejecta mass of 1.38 M\odot, which is kept fixed here, may also vary and in particular involve sub-Chandrasekhar mass WDs (see e.g. Sim et al. 2010). For a fixed \textsuperscript{56}Ni mass, reducing the ejecta mass leads naturally to a significant increase in ejecta ionization (see e.g. Dessart et al. 2012).

**4 DISCUSSION AND CONCLUSIONS**

From this work, we unambiguously discard Na\textsc{i}D as the origin of the 5900 Å feature in SNe Ia after bolometric maximum based on (1) the prediction of [Co\textsc{iii}] 5888 Å line emission from all our delayed-detonation models after bolometric maximum; (2) the strengthening of that [Co\textsc{iii}] line with time in the first two months after bolometric maximum and (3) the satisfactory match of our synthetic spectra to the observations.

This finding is not trivial taxonomy because it further confirms our conclusions from the more theoretical discussion in D13. Although the [Co\textsc{iii}] line was identified three decades ago in nebular phase spectra of SNe Ia (Axelrod 1980) we are discovering the role of [Co\textsc{iii}] in SNe Ia as early as bolometric maximum, and confirming its identification at later times. Lately, a controversial association has been made with Na\textsc{i}D but this association is not supported by models. One explanation for the mis-identification is that [Co\textsc{iii}] lines are not included in the associated radiative transfer calculations (Lentz et al. 2001; Mazzali et al. 2008; Tanaka et al. 2011), as was also done in our earlier modelling of SN Ia. When they are included, the line shows up (Maurer et al. 2011). Another explanation is that SN radiative transfer is often done by separate codes for ‘photospheric’ phase and nebular phase studies, and photospheric codes typically neglect forbidden lines. Unfortunately, this creates a boundary between the two regimes that is artificial. Nebular lines are indeed seen at photospheric epochs, e.g. the [Ca\textsc{ii}] 7300 Å doublet at the end of the plateau in SNe II-P (Dessart et al. 2013c) or [Co\textsc{iii}] 5888 Å early after bolometric maximum (this work). Similarly, strong P-Cygni profiles, typical of photospheric-phase spectra, persist well into the nebular phase.

In the future, we will investigate the radiative properties of SNe Ia as they turn nebular. As shown here, our Chandrasekhar-mass delayed-detonation models exhibit a large range of ionization whereas observations appear somewhat degenerate in that respect. Our simulations differ in \textsuperscript{56}Ni mass but have the same ejecta mass of 1.4 M\odot. While the \textsuperscript{56}Ni mass determines the peak luminosity, the ratio of \textsuperscript{56}Ni to ejecta mass is a key ingredient controlling the ionization state of the gas. Hence, we will investigate whether a range of ejecta masses, tied to a narrow range of \textsuperscript{56}Ni to ejecta mass ratio, can reduce the ionization disparity of our models after maximum.

**ACKNOWLEDGEMENTS**

LD and SB acknowledge financial support from the European Community through an International Re-integration Grant, under grant number PIRG04-GA-2008-239184, and from ‘Agence Nationale de la Recherche’ grant ANR-2011-Blanc-SIMI-5-6-007-01. DJH acknowledges support from STScI theory grant HST-AR-12640.01, and NASA theory grant NNX10AC80G. This work was also supported in part by the National Science Foundation under Grant No. PHYS-1066293 and benefited from the hospitality of the Aspen Center for Physics. AK acknowledges the NSF support through the NSF grants AST-0709181 and TG-AST090074. This work was also granted access to the HPC resources of CINES under the allocation c2013046608 made by GENCI (Grand Equipement National de Calcul Intensif).

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Figure 3. Illustration of the Cobalt ionization state in the inner 20 000 km s\textsuperscript{-1} for our grid of DDC models at 65 d after explosion. Models with a higher \textsuperscript{56}Ni mass systematically show a higher Co ionization level, which is directly connected to a range of spectral colours (bluer for higher \textsuperscript{56}Ni mass; Fig. 1).
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