MULTILAYERED SPECTRAL FORMATION IN TYPE Ia SUPERNOVAE AROUND MAXIMUM LIGHT

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ABSTRACT

We use the radiative transfer code PHOENIX to study the line formation of the wavelength region 5000–7000 Å. This is the region where the SN Ia–defining Si ii feature occurs. This region is important, since the ratio of the two nearby silicon lines has been shown to correlate with the absolute blue magnitude. We use a grid of LTE synthetic spectral models to investigate the formation of line features in the spectra of SNe Ia. By isolating the main contributors to the spectral formation, we show that the ions that drive the spectral ratio are Fe ii, Fe ii, Si ii, and S ii. While the former two strongly dominate the flux transfer, the latter two form in the same physical region inside the supernova. We also show that the naive blackbody that one would derive from a fit to the observed spectrum is very different than the true underlying continuum.

Subject headings: cosmology: miscellaneous — stars: atmospheres — supernovae: general

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1. INTRODUCTION

Type Ia supernovae (SNe Ia) have been used as “standardizable candles” for more than 10 years, thanks to the correlation between their light curve shape and their absolute blue magnitude at maximum light. This correlation is well matched by a spectroscopic sequence (Nugent et al. 1995) defined by the ratio $R_{Si}$ of the depth of two absorption features usually identified as Si ii 6352 and 6355 lines. Using the radiative transfer code PHOENIX (Hauschildt & Baron 1999; Baron & Hauschildt 1998; Hauschildt et al. 1996, 1997a, 1997b, and references therein), this sequence has been matched to a temperature sequence that could physically be related to the amount of $^{56}$Ni produced in the context of Chandrasekhar-mass white dwarf explosions. Hatano et al. (2000) showed that $R_{Si}$ and the velocity derived from the minimum of the $\lambda 6100$ feature correlated poorly, suggesting that a one-parameter description of SNe Ia was insufficient. This velocity derived from the P Cygni feature associated with the Si ii 6355 line and its time evolution break SNe Ia into subclasses depending on more than one parameter (Benetti et al. 2005). Branch et al. (2006) and Hachinger et al. (2006) also showed that different spectroscopic indicators exist that can be used to distinguish variations even within the “normal” SNe Ia. In the context of Chandrasekhar-mass explosions, these variations cannot be interpreted only in terms of differences in the amount of $^{56}$Ni produced. The velocity scatter could be due to properties of the progenitor system that impact the kinetic energy released during the explosion. For example, the ratio ($^{54}$Fe + $^{56}$Ni)/$^{56}$Ni has been proposed as a second physical parameter that could account for this dispersion (Mazzali & Podsiadlowski 2006).

This paper is an attempt to unravel the spectral formation in the 5000–7000 Å region (henceforth the $R_{Si}$ wavelength region), as a way to address the physical reasons for their correlation with luminosity and especially the link between this correlation and the temperature sequence of SNe Ia. A previous attempt using the radiative transfer code SYNOW (Fisher 2000) was performed by Garnavich et al. (2004), who explained the counterintuitive correlation of $R_{Si}$ with luminosity by the temperature sensitivity of a Ti ii line. On the other hand, synthetic spectral investigations (Stehle et al. 2005; Branch et al. 2006) failed to find any important Ti ii line contributions in this part of the spectrum.

We use the radiative transfer code PHOENIX differently than it has usually been used. Instead of fitting a supernova by varying the time and bolometric luminosity, we use a grid of simulated models to probe the line formation process. Our input model is the parameterized deflagration model W7 (Nomoto et al. 1984), homologously expanded to calculate the abundances at any given time. The knowledge of the abundance structure of the explosion model, together with the self-consistent physical structure provided by PHOENIX, are used to describe more precisely how the spectrum is formed in SNe Ia. Bongard et al. (2006) introduced the line ratio $R_{SiS}$, which is defined as the ratio of two integrals of the flux over a chosen wavelength range, where each integral is centered around the two lines used in the original definition of $R_{Si}$ (see § 6.1). It is designed to be useful for spectra that have lower signal-to-noise ratio than well-observed nearby SNe Ia.

This understanding of the formation of the spectrum allows us to explain why the line ratio $R_{SiS}$ is a good probe of the temperature sequence and reinforces the link between this sequence and the absolute blue magnitude of SNe Ia. These results also allow us to rule out a Ti ii contribution to the correlation of $R_{Si}$ with luminosity. We emphasize that even though the synthetic spectra presented here do not do a good job of reproducing observed SN Ia spectra, we consider W7 to be the fiducial SN Ia model. Baron et al. (2006) showed that reasonably good synthetic spectra can be produced with W7 near maximum light. We make differential comparisons based on that model, keeping in mind that Baron et al. (2006) emphasized that W7 did not reproduce the wavelength region that we examine in detail here.
We address time evolution only qualitatively. The goal of this paper is to understand the temperature sequence of SN Ia spectra around maximum light; thus we concentrate on day 20 after explosion, since maximum light in B in SNe Ia has been shown to occur 18–25 days after explosion.

2. ANALYSIS TOOL: PHOENIX SIMULATIONS

2.1. The LTE Grid

Using the multipurpose radiative transfer code PHOENIX, we converged LTE calculations for the W7 explosion model at 10, 15, 20, and 25 days after explosion, for a range of bolometric luminosities spanning the “normal” supernova blue magnitudes.

2.2. Single-Ion Spectra

Each model converged with PHOENIX provides not only a spectrum but also knowledge of the physical structure and line optical depth in the supernova. This gives us the ability to compute “single-ion spectra” as follows. Using the converged output of the PHOENIX simulation, we artificially turn off all but the continuum and one single-ion line opacities. The “continuum opacities” denote all the bound-free and free-free opacities, as well as electron and Rayleigh scattering. We then recalculate the solution of the scattering problem in order to get the “single-ion spectrum,” with the level populations and free electron number kept fixed.

The relative strength of the absorption and emission features in this spectrum give an indication of the contribution of each line to the complete spectrum. Since the solution of the scattering problem is recalculated, the features are not expected to look exactly the same as in the complete spectrum. In any case, due to the global nature of the transfer equation, the full spectrum is not the linear combination of all the single-ion spectra.

In these single-ion spectra, the flux transfer from the blue to the red due to scattering will be smaller, due to the opacity decrease caused by the suppression of most of the ions. They will thus appear bluer than the complete spectrum. The backscattering will also be decreased for the same reason, resulting in “single-ion spectra” brighter than the full synthetic spectrum.

The ratio of scattering to absorption is larger in the single-ion spectra than in the full synthetic spectrum, because the full scattering problem is solved with fixed level populations and fewer atomic lines. The same effect enhances stimulated emission in the single-ion spectra, resulting in strong net emission in the P Cygni profiles.

Since the single-ion spectra are always brighter than the full synthetic spectrum, we must normalize the luminosity in order to compare the two spectra. We do this by setting the single-ion atomic lines. The same effect enhances stimulated emission in the single-ion spectrum, with the level populations and free electron number kept fixed.

3. USING SINGLE-ION SPECTRA: RULING OUT

3.1. The R_{Si} Puzzle

Because of their similar redshift with respect to Si II λ6355 and Si II λ5972 lines, it is tempting to consider the 6100 and 5800 Å troughs to be part of their P Cygni profiles. These two lines share the 4P level; the λ6355 line is the 4S–4P transition and the λ5972 line is the 4P–5S transition. Their optical depths can thus be estimated in the Sobolev approximation using (Hatano et al. 1999)

\[ \tau = \frac{\pi e^2}{mc} f \Delta E_{nl} \left( 1 - \frac{q_l n_l}{q_u n_u} \right), \]

where \( n_l \) and \( n_u \) are the number densities of the lower and upper level associated with the transition, \( f \) is its oscillator strength, \( t \) is the time since explosion, \( q_l \) and \( q_u \) are the statistical weights of the levels, and \( \Delta E \) is the wavelength of the transition. Assuming thermal equilibrium, the ratio of the Si II λ6355 line optical depth (\( \tau_{red} \)) to the Si II λ5972 line optical depth (\( \tau_{blue} \)) becomes

\[ \frac{\tau_{red}}{\tau_{blue}} \propto \frac{(1/3)e^{\Delta E_{red}/(kBT)}}{1 - 3e^{-\Delta E_{blue}/(kBT)}}, \]

where \( \Delta E \) is the energy difference between the upper and lower levels of the transition. This ratio decreases monotonically with respect to a temperature increase, as also shown in Figure 1, where SYNOW was used to compute Si II spectra for excitation temperatures ranging from 5000 to 40,000 K.

Since P Cygni troughs become deeper with increasing optical depth, a higher Si II excitation temperature should increase \( R_{Si} \). Under the reasonable assumption that higher luminosity SNe Ia have higher Si II excitation temperatures, \( R_{Si} \) should increase and not decrease with luminosity. However, observations show the opposite behavior.

Figure 2 displays the temperature structure from our grid of calculations 20 days after explosion with increasing bolometric luminosities. We restricted the plot to the 9000–16,000 km s^{-1} region, where silicon is found in W7. This shows the physical temperature increases with bolometric luminosity, as one would expect. However, a temperature structure inversion in the 9000–16,000 km s^{-1} region due to non-LTE (NLTE) effects, Si II lines alone are
unable to explain the trend of the \( R_{Si} \) correlation with SN Ia blue magnitude.

3.2. Ti \( \Pi \) Impact on the \( R_{Si} \) Wavelength Region

Garnavich et al. (2004) proposed that \( R_{Si} \) variation with luminosity could be accounted for by a blend of Ti \( \Pi \) lines. We focus on the behavior of the \( \lambda 6013 \) line. Garnavich et al. (2004) suggested that the \( R_{Si} \) puzzle described above could be solved by the temperature evolution of this line, which increases much faster than the Si \( \Pi \) \( \lambda 5972 \) line decreases below 7000 K.

In order to probe this assumption, we display in Figure 3 the day 20 two-ion spectra of Si \( \Pi \) and Ti \( \Pi \) alone, as well as the full spectrum for our lower luminosity model. We also display the continuum-only spectrum as a reference. For Si \( \Pi \), the 6100 Å trough and the concomitant emission peak are, as expected, dominated by Si \( \Pi \) lines, but the Si \( \Pi \) \( \lambda 5972 \) P Cygni profile lacks the full-spectrum blue edge, hinting at a missing contribution to the full-spectrum line profile. This other contribution cannot be Ti \( \Pi \), as no Ti \( \Pi \) lines appear in the \( R_{Si} \) wavelength region, even though the Ti \( \Pi \) \( \lambda 6013 \) line has been checked to form between 12,000 and 16,000 km s\(^{-1}\), where the temperature is below 7000 K, as indicated by the black line in Figure 2.

One could argue that this line does not appear in our two-ion spectrum because of a too low abundance of titanium in W7. We rule out the low abundance in W7 from the Si \( \Pi \) single-ion spectrum shows a strong feature to the blue of 5000 Å, which does a reasonably good job of reproducing the observed trough seen in fast decliner SNe Ia such as SN 1991bg.

Figure 2 shows the PHOENIX temperature structure between 10,000 and 16,000 km s\(^{-1}\), where the Si \( \Pi \) and Ti \( \Pi \) lines of the \( R_{Si} \) wavelength region form in all our synthetic spectra models. Using SYNOW, we were able to fit the \( R_{Si} \) wavelength region with Si \( \Pi \) and Ti \( \Pi \) lines alone, but required a Ti \( \Pi \) excitation temperature of 40,000 K. This temperature is way too high compared to the detailed PHOENIX results, but note that the temperature in SYNOW is dependent on the chosen reference line. However, even with SYNOW, one expects that Ti \( \Pi \) line strength increases with decreasing temperature. What is happening in this case is that in order to obtain a noticeable contribution of Ti \( \Pi \) (with respect to Si \( \Pi \)), we must go to very high excitation temperatures combined with extremely large optical depths in Ti \( \Pi \):

the temperature dependence is not independent of the Ti \( \Pi \) optical depth, which in SYNOW is a free parameter.

This very high excitation temperature does not necessarily indicate that the assumptions of SYNOW have broken down, since the PHOENIX and SYNOW Ti \( \Pi \) spectra agree quite well for similar temperatures. In Figure 4 we display the comparison between the SYNOW results and the PHOENIX results in the temperature range appropriate to the physical results from PHOENIX. The Si \( \Pi \) and the Ti \( \Pi \) line strengths agree. We also agree with the point of Garnavich et al. (2004) that the temperature dependence of the strength of Ti \( \Pi \) is such that the line strength increases dramatically below 7000 K; however, the relative strength of the line with respect to Si \( \Pi \) does not increase fast enough for the Ti \( \Pi \) line to become important at reasonable physical temperatures. This is due to the fact that the initial line strength of Ti \( \Pi \) is so small.

4. MULTILAYERED SPECTRUM FORMATION

4.1. The Deepest Layer

The multilayer spectrum formation picture alters the way that one thinks about how spectrum formation occurs. In the photospheric picture, one thinks about features forming in a reversing layer above a true continuum. In the multilayer picture, features can form throughout the supernova atmosphere and can in principle imprint a shape into the “continuum” that is altered higher up in the atmosphere. The most important difference between the multilayer picture and the photospheric picture is that features from multiple ionization stages can strongly affect the overall spectrum.

In the top panel of Figure 5, we display the deepest layer of the spectral formation of our lower bolometric luminosity model: the continuum-only spectrum. It forms below 3000 km s\(^{-1}\) for all our range of bolometric luminosities, where the continuum optical depth becomes greater than 1, which is at a much lower velocity than where the photosphere is usually considered to be in the photospheric model.

The bottom panel of Figure 5 clearly shows that the naive blackbody fit (that is, the blackbody that peaks at the same wavelength as the smoothed full synthetic spectrum) to the full synthetic spectrum would give a blackbody temperature that is much cooler than the true underlying continuum. While the continuum-only spectrum is brighter and bluer (as described in § 2.2), the bottom panel of Figure 5 shows that the blackbody
obtained from the physical temperature 13,685 K is also significantly bluer than the naive blackbody. This is a very important point, since it shows that the naive blackbody has nothing to do with the real physical conditions.

It is crucial to keep this point in mind when analyzing SN Ia features, especially when using techniques such as principal component analysis (PCA; James et al. 2006). It is tempting to subtract a “continuum” case by case in order to maximize the contribution of the lines. Since the “pseudocontinuum” is responsible for a large part of the spectral structure, this procedure yields the opposite result: the subtracted “continuum” adds a fake relationship between features. The PCA eigenvectors will thus no longer account only for real SN Ia diversity, but also for the arbitrary continuum.

The blackbody in the bottom panel of Figure 5 corresponds to the temperature at which $T_{\text{eff}} = 13,685$ K. Even at depth of 2000 km s$^{-1}$ ($T_{\text{eff}} = 13,685$ K), the supernova spectrum is not a blackbody spectrum. The spectrum of the full W7 model is obtained from the steep narrow blue continuum-only spectrum by line interactions that transfer flux toward the red by Doppler shift or fluorescence.

### 4.2. Iron Lines

In Figure 6 we display the Fe II, Fe III, and Fe II+Fe III two-ion spectra of our faintest model at day 20. The $R_{\text{Si}}$ wavelength region (5000–7000 Å) gives us some insight into the spectral formation process because of the smaller number of strong lines than in the bluer spectral regions. The Fe III and the Fe II peaks at 5900 and 6100 Å are blends of weak lines formed at velocities of ~5000 and ~9000 km s$^{-1}$, respectively. It follows from the optical depths shown in Figure 7 that the 5128 Å Fe II peak and the 5170 Å Fe II peak arise from strong lines formed at velocities of ~7000 and ~15,000 km s$^{-1}$, respectively.

Figure 6 shows how Fe III and Fe II lines blend together. The strong Fe III 5128 Å feature is shielded by the strong Fe II 5170 Å one, and the two blends above 5900 Å merge.

In the photospheric model, the spectrum is considered to be a blackbody continuum emitted by the photosphere on top of which strong, well-separated lines of ions present in the line-forming region add structure mainly by scattering light. We define the “pseudocontinuum” as the spectrum formed by weak line blends, which produces more structure than a blackbody spectrum. The photosphere is replaced in this picture by a “pseudophotosphere.”
forming at a depth depending on wavelength. This concept is widely used in the radiative transfer community.

This pseudophotosphere is clearly seen in the results of Branch et al. (2005), who were able to model the spectrum of the normal SN Ia 1994D using SYNOW at 115 days past maximum light, at least in the blue. Specifically, the results of Branch et al. (2005) show that even at late times (thus in the deepest layers) the spectrum is dominated by permitted lines that can be treated in resonant scattering.

Similarly, the line-forming region of the pseudophotospheric model does not have a fixed depth. We define it as the region where the strong lines that create the final structure of the spectrum form. In this picture, the strong Fe II 5128 Å feature does not belong to the line-forming region because it forms in the continuum only, well below the Fe II feature.

The Fe II+Fe III spectrum we display in Figure 6 can be considered to be the pseudocontinuum spectrum in the 5000–7000 Å region. It is formed by a large peak due to Fe II 5128 Å and neighboring strong Fe II lines, followed by a flat region forming between 5000 and 9000 km s⁻¹, depending on wavelength. This shows that by construction, R Si couples spectral regions that form at very different depths.

In the pseudophotospheric model, the flux transfer from the blue to the red is dominated by Fe III and Fe II weak line blends. Of course, weak cobalt and nickel lines also contribute, but the study of their effects will be postponed to a later paper in which more complicated spectral formation in the λ < 5000 Å region will be discussed. The colors of SNe Ia are therefore dominated by weak lines of the heavy elements whose blending shapes the pseudophotosphere spectrum.

5. IRON LINES AND COLORS

As the bolometric luminosity of our models is increased, the temperature also rises, ionizing Fe II to Fe III. The Fe II number abundance depletion decreases the 5170 Å feature strength, leaving S II the dominant ion of the blue edge of the R Si feature at ~5455 Å. This effect can be seen in Figures 8–10, where the Fe III, Fe II, Si II, and S II spectrum changes with bolometric luminosity are displayed. The Fe II 5170 Å feature strength decreases as Fe II is ionized into Fe III, unshielding the strong Fe III 5128 Å feature. Simultaneously, the flux transfer toward the red decreases, because Fe II is much more efficient at transferring flux toward the red than Fe III, as can be seen in Figure 6. This efficient flux transfer from the blue to the red is due to numerous blue and UV Fe II lines that amount to a large opacity because of line blanketing.

Figure 6 also shows that in the 5000–8000 Å wavelength region, Fe III features remain very stable over the range of bolometric luminosities explored, while Fe II features vary much more. This is not surprising, as Fe II lines form much deeper, in a region that is hotter and denser, where physical conditions vary less than in the outer regions.

We see in the top panel of Figure 9 that the Fe III+Fe II two-ion spectrum undergoes a strong increase of flux below 5500 Å, while it remains very stable above, when the bolometric luminosity increases. This translates into a strong variation in color.
of the full synthetic spectrum. On the other hand, the Si $\text{ii} + \text{S} \text{ii}$ two-ion spectra displayed in the bottom panel of Figure 9 remain very consistent in shape, while their flux follows the continuum-only spectrum flux increase.

The flux variation displayed in Figure 10 is thus dominated by the "pseudocontinuum" of Fe $\text{iii}$ and Fe $\text{ii}$ lines, especially the weak line blends, on top of which the strong Si $\text{ii}$ and S $\text{ii}$ lines add structure. The flux transferred by the well-separated lines formed in the line-forming region is small compared to the flux transferred at depth by iron lines, but is by no means negligible when using SNe Ia for precision cosmology. It is therefore crucial to have a good description of the full spectrum in order to perform $K$-corrections.

Figure 14 shows very close agreement between the full synthetic spectrum and the Fe $\text{iii} + \text{Fe} \text{ii} + \text{Si} \text{ii} + \text{S} \text{ii}$ four-ion spectrum above 5000 Å, proving that in the W7 model the other metallic lines have a secondary importance in transferring flux compared to Fe $\text{iii}$ and Fe $\text{ii}$ lines. Faint SNe Ia are expected to be redder because of a larger proportion of Fe $\text{ii}$ (compared to Fe $\text{iii}$) and not because the underlying naive blackbody is colder. That is, accepting that the primary variation for the peak luminosity is due to nickel mass (Nugent et al. 1995), dimmer supernovae are redder because the underlying ionization stage is primarily Fe $\text{ii}$.

Figure 11 clearly displays this brighter, bluer evolution for each epoch we simulated.

While the variation with epoch is beyond the scope of this work, the variation with luminosity in part mimics the variation with epoch to some extent. Moreover, the spectra at 10 days after explosion are much bluer than the later ones, because the supernova is much denser and hotter at this epoch, leading to a higher degree of ionization of the iron core.

This Fe $\text{iii} -\text{Fe} \text{ii}$ effect on flux transfer agrees with the analysis of Kasen (2006), which explains the second red bump in SN Ia.

![Figure 8](image1.png)  
**Fig. 8.—** Fe $\text{ii}$ (top) and Fe $\text{iii}$ (bottom) day 20 single-ion spectra as a function of $M_{\text{bol}}$. Each spectrum is rescaled to the bolometric flux of the corresponding full synthetic spectrum. Since Fe $\text{iii}$ forms deeper, it is less sensitive to a change in the bolometric luminosity. Fe $\text{ii}$ lines are more efficient at transferring flux from blue to red. [See the electronic edition of the Journal for a color version of this figure.]

![Figure 9](image2.png)  
**Fig. 9.—** Fe $\text{ii} + \text{Fe} \text{iii}$ (top) and Si $\text{ii} + \text{S} \text{ii}$ (bottom) two-ion day 20 spectra as a function of $M_{\text{bol}}$. The flux transfer from the blue to the red is dominated by the iron (and other iron peak elements in the full spectrum). All spectra are rescaled to have the same flux as the corresponding full synthetic spectra. [See the electronic edition of the Journal for a color version of this figure.]

![Figure 10](image3.png)  
**Fig. 10.—** Fe $\text{iii} + \text{Fe} \text{ii} + \text{Si} \text{ii} + \text{S} \text{ii}$ four-ion day 20 spectra as a function of $M_{\text{bol}}$. [See the electronic edition of the Journal for a color version of this figure.]
light curves by the change in opacity due to the recombination of Fe\textsc{iii} into Fe\textsc{ii}: when the temperature decrease in the SN Ia envelope is enough for Fe\textsc{iii} to recombine into Fe\textsc{ii}, more flux is transferred from the blue into the red, causing the second red bump.

5.1. Silicon and Sulfur Lines

The top panel of Figure 12 displays the Fe\textsc{ii}+Fe\textsc{iii} two-ion spectrum and the Si\textsc{ii} single-ion spectrum. Si\textsc{ii} lines form in the line-forming region, contributing little to the global flux transfer, but adding lots of structure to the spectrum. As previously mentioned, the \( \lambda 6100 \) trough, as well as the Si\textsc{ii} \( \lambda 6355 \) emission peak, is dominated by a strong Si\textsc{ii} line. The Si\textsc{ii} \( \lambda 5972 \) line is also seen to dominate the second P Cygni trough, but Si\textsc{ii} alone fails to account for the blue edge at \( \lambda 5600 \). We already ruled out Ti\textsc{ii}, and the Fe\textsc{ii} \( \lambda 5170 \) peak is too blue to account for this edge. The bottom panel of Figure 12 displays the S\textsc{ii} single-ion spectrum in addition to the previous ones, showing that S\textsc{ii} lines can account for the bluer edge of the R\textsc{Si} wavelength region.

The Si\textsc{ii}+S\textsc{ii} two-ion day 20 spectra (top, not rescaled; bottom, rescaled, Fe\textsc{ii}+Fe\textsc{iii} and Si\textsc{ii}+Fe\textsc{ii}+Fe\textsc{iii} are also shown). [See the electronic edition of the Journal for a color version of this figure.]

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The Si\textsc{ii}+S\textsc{ii} spectrum in the top panel of Figure 13 shows that the relative strengths of the peaks and depths due to Si\textsc{ii} and S\textsc{ii} in the R\textsc{Si} wavelength region are consistent with the spectrum of the full W7 model. In the bottom panel of Figure 13, where all the spectra are rescaled to have the same total flux, if the R\textsc{Si} line features are dominated by Si\textsc{ii} and S\textsc{ii}, it is the Fe\textsc{iii} and Fe\textsc{ii} lines that provide the flux background. The Fe\textsc{iii}+Fe\textsc{ii}+Si\textsc{ii}+S\textsc{ii} spectrum shows that between 5000 and 8000 \( \AA \) the spectrum of the full W7 model is well reproduced by these four ions alone. This is an important result for understanding the theoretical explanation of the correlation between the line ratios and the absolute B magnitude. Since we have shown that the R\textsc{Si} ratio (that is, the flux in this wavelength range) depends only on the iron, silicon, and sulfur, to correctly model the line ratio, one must only have a model that correctly accounts for these ions.
Clearly, we are not there yet, but this result significantly reduces the parameter space that must be studied to obtain physical understanding.

However, we must be cautious because our models do not reproduce the observed spectra. For example, W7 does not reproduce the shape of the Si ii 6100 Å feature (Baron et al. 2006), and thus we could be missing at least one important species in our calculations. Turning this around shows that finding the correct variation of $R_{\text{SiS}}$ with luminosity could be an important filter for obtaining physically correct models.

Similarly, the strong iron features around 4500 and 5170 Å are unrealistically large compared to observed spectra. These strong features are a finer probe of the quality of a model than the overall shape of the spectrum: the thick blend of lines of the iron core is much less sensitive to an abundance variation than the strong lines, forming where the iron blanket has become optically thin.

6. $R_{\text{SiS}}$: OBSERVATIONAL SUPPORT OF THE MULTILAYERED SPECTRAL FORMATION

6.1. $R_{\text{SiS}}$ Predicted Trend: A Hotter PHOENIX Spectrum

We defined a line ratio $R_{\text{SiS}}$ (Bongard et al. 2006) as

$$ R_{\text{SiS}} = \frac{\int_{5700}^{5500} F_{\lambda} \, d\lambda}{\int_{6200}^{6450} F_{\lambda} \, d\lambda}. $$

We showed that it was better correlated to luminosity than $R_{\text{Si}}$ and deferred the motivation to the present paper. Here we address this question.

As shown in the previous sections, the $R_{\text{Si}}$ wavelength region is dominated by Fe iii, Fe ii, Si ii, and S ii lines. Moreover, for luminosities corresponding to “normal” SNe Ia, the bluer edge of this wavelength region is dominated by Si ii, since the envelope is still too hot to allow the strong Fe ii 5170 Å feature to dominate. As the luminosity decreases, the strength of the Fe ii 5170 Å feature increases; this behavior is illustrated in Figure 14. This effect will have differing importance for the two different definitions of the line ratio, $R_{\text{Si}}$ and $R_{\text{SiS}}$. $R_{\text{Si}}$ will hardly be affected, since the depth of the blue Si ii feature does not vary significantly; however, $R_{\text{SiS}}$ uses just this wavelength region and will thus be strongly impacted by the growth of the Fe ii 55170 line.

The “multilayered line formation” picture shows that the depth of the troughs are not the pertinent quantities to probe the temperature sequence, since the “absorption” features are formed by a complex blend of absorptions and emissions due to ions spanning a wide range of depth. The intermediate ~5900 Å $R_{\text{Si}}$ peak has the same problem, as it is a blend of Fe iii, Fe ii, and Si ii lines. A direct corollary is that $R_{\text{SiS}}$ does not measure line strength evolution, as is commonly believed.

The motivation for the definition of $R_{\text{SiS}}$ was to isolate contributions from Si ii and S ii lines forming in the same physical region between 10,000 and 15,000 km s$^{-1}$. There are at least two options for the correlation of $R_{\text{SiS}}$ with absolute blue magnitude: the silicon and sulfur lines form in the same physical region and their strength is simply determined by the local conditions, or more likely, $R_{\text{SiS}}$ does not measure the region where silicon and sulfur lines form, but rather the conditions where the iron “pseudocontinuum” forms.

Keeping in mind that one should be careful when interpreting single-ion spectra, Figure 9 supports this latter explanation. The top panel of Figure 9 shows that the Fe ii and Fe iii blend varies little in the 6100 Å wavelength zone used to compute $R_{\text{SiS}}$. The consistency in the Si ii + S ii two-ion spectra shape displayed in the bottom panel of Figure 9 suggests a small variation of the relative strength of the Si ii and S ii features. We therefore favor...
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The change in slope between day 20 and day 25 days after explosion is due to Fe trends of real and synthetic spectra for 20 and 25 days after maximum are similar. We used a grid of LTE PHOENIX synthetic spectra using the W7 model to study the spectral formation in SNe Ia around the time of maximum light. Instead of focusing on fitting synthetic to observed spectra, we probed the detailed line formation in the synthetic spectrum to try to understand which ion was responsible for which feature, while taking detailed line blending into account.

We analyzed the synthetic spectra in detail to study the line formation in the $R_{\text{Si}}$ wavelength region, showing that the $\lambda 6355$ peak and the 6100 $\AA$ trough were dominated by Si ii lines forming over a blend of Fe ii and Fe iii lines. The intermediate 5800 $\AA$ peak has been shown to be a complex blend of Si ii $\lambda$6355, Si ii $\lambda$5972, Fe iii, and Fe ii weak lines. The Ti ii contribution to the 5500 $\AA$ trough has been ruled out. We showed that the redder edge was dominated by the Si ii $\lambda$5972, line, whereas the bluer one was dominated by the Si ii $\lambda$5455 line or the Fe ii $\lambda$5170 line, depending on luminosity. Based on our unraveling of the line formation in this wavelength region, we are able to illustrate our motivation for the definition of $R_{\text{SiS}}$, isolating the Si i and S ii contributions of the $R_{\text{Si}}$ region.

We described a multilayer model in which the observed pseudocontinuum is formed throughout the entire supernova, and thus strong features from multiple ionization stages can occur in the observed spectrum. We stress the importance of the numerous weak iron lines and show that their blends dominate the flux transfer. As a corollary, in the multilayer model, the inner spectrum is not close to a Planck function, but contains much more structure background. We showed that the ionization stage of the iron core dominates the SN Ia colors, explaining the brighterbler relation at maximum light. Even though a detailed study of time evolution is beyond the scope of this paper, we show that our results are also qualitatively consistent in this regard, our earlier spectra being systematically much bluer than our later ones.

6.2. Synthetic versus Observed Spectra

Up to now, we have used the W7 model as a reasonable physical explosion model of SNe Ia, but we did not try to match observed spectra. We used the knowledge of the abundance structures and the physical structure obtained by PHOENIX to probe the line formation process, considering the W7 model a theoretical supernova of which we had complete knowledge.

The $R_{\text{SiS}}$ ratio correlates well with absolute blue magnitude (Bongard et al. 2006). In Figure 15 we display $R_{\text{Si}}$ and $R_{\text{SiS}}$ for our day 20 and day 25 models, as well as real SN Ia data. The calculated $R_{\text{Si}}$ appears to reproduce the observed data quite well for both days 20 and 25. It follows the “normals” quite well and may even extend to the regime of very low luminosity SNe Ia, such as SN 1991bg. At first glance, it would appear that the calculated $R_{\text{SiS}}$ fails to match the observations; however, if one restricts one’s attention to the “normals” (Fig. 15, bottom), in fact the agreement between $R_{\text{SiS}}$ (for day 25) and the data is better than that for $R_{\text{Si}}$. The change in slope we observe around $M_B = -19.1$ for day 25 comes from the strong Fe ii $\lambda 5170$ $\AA$ feature, which dominates over S ii at lower luminosities. It should be noted that the W7 model is not expected to reproduce SN Ia light curves and certainly cannot be expected to match the observed diversity from fast to slow decliners. Therefore, the time since explosion should be considered only indicative and related only with great care to real supernova epochs.

7. CONCLUSION

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