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IONIZATION OF TYPE Ia SUPERNOVAE: ELECTRON IMPACT, PHOTON IMPACT, OR CHARGE TRANSFER?

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ABSTRACT

The ionization structure of the nebular Type Ia supernova iron core is determined by treating important atomic processes with the best available evaluated atomic data and by assuming both Chandrasekhar–mass and sub-Chandrasekhar-mass white dwarf explosion models. The electron impact ionization rates are calculated by analyzing the energetic electron energy deposition processes. Charge transfer processes between neutral and ionized iron-group elements are included in the calculations using the recently available rate coefficients. The effect of photoionization due to the recombination photons is critically evaluated by carrying out a detailed cascade calculation using the recently improved state-specific rate coefficients of radiative recombination and cross sections of photoionization of iron. It is concluded that the ionization structure is mainly controlled by a combination of the energetic electron impact ionization and charge transfer, while the photoionization plays only a minor role and its effect on the synthetic spectra is small.

Subject headings: atomic data — atomic processes — supernovae: general

1. INTRODUCTION

In comparison with Type II supernovae, Type Ia supernovae (SNe Ia) are characterized by a much higher state of ionization as a result of both the synthesis of larger masses of radioactive materials and the lower gas densities. Through determination of their ionization structure, we have constructed synthetic spectra to compare with the nebular spectra of SNe Ia (Liu, Jeffery, & Schultz 1997a, 1997b). These investigations have led to strong constraints on the explosion models of SNe Ia, and they favor the density profiles and elemental compositions of the iron core predicted by sub–Chandrasekhar-mass white dwarf (WD) models over those predicted by the currently available Chandrasekhar-mass WD models. This conclusion has been reached based on an ionization model of SNe Ia that treats important atomic processes with reliable atomic data. These processes include energetic electron impact, charge transfer, radiative and dielectronic recombination, photoionization due to the photons emitted in recombination to the ground and low-lying metastable states of the product ions, radiative processes, and thermal electron collisional processes. In comparison with the electron impact and charge transfer, photoionization due to recombination to the more highly excited states is less important mainly because the recombination goes through such a complicated cascading process that the production rate of photons which are energetic enough for photoionization is much less than the total recombination rate.

We have included these photoionization processes in our more recent calculations (Liu et al. 1997c) by carrying out a detailed cascade analysis using the recently improved state-specific recombination rate coefficients (Nahar 1996b, 1997; Nahar, Bautista, & Pradhan 1997) and photoionization cross sections (Nahar & Pradhan 1994; Nahar 1996a; Bautista 1997). Our calculations demonstrate that the ionizing photons come mainly from recombination to the ground and low-lying metastable states and that only a small fraction of them originate in the recombination to the more highly excited states and in the subsequent cascade. We conclude that the photoionization is less important than a combination of the energetic electron impact ionization and charge transfer and its effect on the synthetic spectra is minor. Thus our previous conclusion on the explosion models of SNe Ia is strengthened (Liu et al. 1997a, 1997b).

2. IONIZATION MODEL

Ionization of SNe Ia at about 300 days since the supernova explosion is mostly driven by the radioactive decay of ^{56}Co which is the decay product of the explosively synthesized ^{56}Ni and deposits energy in the form of γ-rays and positrons. Annihilation of the positrons also produces γ-rays. The γ-rays lose energy in Compton scattering with free and bound electrons and are degraded into X-rays and produce energetic electrons. The energy deposition of the γ-rays was calculated using the gray-atmosphere transfer approach of Swartz, Sutherland, & Harkness (1995), and the kinetic energy of the positrons was assumed to be deposited locally to produce fast electrons. The method is physically reasonable and computationally efficient, and the γ-ray energy deposition rates are considered to be accurate to within about 10% which is generally lower than the uncertainties of the atomic data. The X-rays are absorbed in inner-shell ionizations of iron-group elements to produce fast electrons. Only the total rate of energy input by the radioactive decay is needed in the ionization calculation because the result does not depend on the actual high-energy photon energy distribution (Liu & Victor 1994).

These energetic electrons lose energy in ionizing and exciting the atoms and ions and in heating the gas via the Coulomb collisions with the thermal electrons. We have analyzed the fast electron energy deposition processes in the iron core using the best available cross section data (Lennon et al. 1988; Freund et al. 1990; Pradhan & Berrington 1993; Zhang & Pradhan 1995) and by treating the degradation of the secondary electrons using a Monte Carlo approach (Liu & Victor 1994). This approach has been employed to explore the chemistry of SNe Ia and successfully explain the undetectability of molecules in SNe Ia (Liu 1997, 1998). The electron impact ionization rates are given by the rate of energy input by the radioactive decay divided by the mean energies per ion pair. In a highly ionized iron gas, the mean energies depend on the fractional abundances of the ions and electrons, and they are several tens of the corresponding ionization potentials.

The ionization distribution among the iron-group ions is significantly affected by charge transfer of the ions with the neutral atoms. We have included these charge transfer reactions using the recently calculated rate coefficients of $7.1 \times 10^{-9}(T/10^4\ \mathrm{K})^{0.43}$, $1.2 \times 10^{-8}(T/10^4\ \mathrm{K})^{0.43}$, and $1.6 \times 10^{-8}(T/10^4\ \mathrm{K})^{0.43}\ \mathrm{cm^3\ s^{-1}}$ for the charge transfer from Fe^+, Fe^{2+}, and Fe^{3+}, respectively, to Fe, where T is the temperature (Krstić, Stancil, & Schultz 1997). Charge transfer processes involving higher charge states are unimportant because of the relatively low abundances of these highly charged ions in SNe Ia. These rate coefficients are higher by orders of magnitude than the rate coefficients of the corresponding recombination processes between the ions and electrons that are of the order of $10^{-12}\ \mathrm{cm^3\ s^{-1}}$ at several thousand kelvins (Nahar 1996b, 1997; Nahar et al. 1997), though the rates of charge transfer and recombination are closer when the neutral abundance is many orders of magnitude below unity. It should be noted that these recently calculated recombination rate coefficients are much higher than the previous estimates by Woods, Shull, & Sarazin (1981), which had been used in similar calculations prior to Liu et al. (1997a).

Recombination of a higher-charged iron ion can produce photons energetic enough to ionize a lower-charged ion through a direct or cascading process. We have carried out a detailed analysis of the cascading process using the recently improved state-specific recombination rate coefficients (Nahar 1996b, 1997; Nahar et al. 1997). We included all the relevant observed and calculated energy levels of the product ions in our cascade calculations. We assumed that the highly excited hydrogenic states with $n > 10$ cascade in a manner similar to that for the recombination of free electrons. We found that at 6000 K, about 16%, 15%, and 60% of the recombination from Fe^{3+} to Fe^{2+} produce photons energetic enough to ionize Fe^{2+}, Fe^+ but not Fe^{2+}, and Fe only, respectively. These percentages become, respectively, about 14%, 12%, and 61% at 4000 K and about 17%, 18%, and 61% at 8000 K. The percentages of the recombination from Fe^{2+} to Fe^+ which produce photons energetic enough to ionize Fe^+ and Fe only are about 12% and 20%, respectively, from 4000 to 8000 K. The photoionization rates were estimated by adopting an escape probability approach using the photoionization cross sections presented by Nahar & Pradhan (1994), Nahar (1996a), and Bautista (1997). This approach is adequate because the photoionization is less important than the combination of the fast electron impact ionization and charge transfer, as demonstrated by the results presented below. Photoionization of the abundant species is essentially a local process because the high optical depths result in predominantly local absorption of the ionizing photons. For much less abundant species such as neutral Fe for model SC and in the outer region for model W7, photoionization is not very important because of the optically thin condition. Although charge transfer processes may also produce ionizing photons, their effects on photoionization are likely to be smaller than those due to recombination.

Because the atomic reaction timescales are much shorter than the supernova expansion timescale and the radioactive decay timescale, the ionization and thermal structure is in a steady state. We have constructed a steady state model of the ionization structure of SNe Ia based on the atomic processes discussed above. The temperature was self-consistently calculated by balancing the heating and cooling rates using the best available radiative and collisional data described by Liu et al. (1997a). It is of the order of few thousand kelvins at 300 days.

Two representative models of SNe Ia were examined: (1) the carbon deflagration Chandrasekhar-mass model W7 (Thielemann, Nomoto, & Yokoi 1986) for a 1.38 $M_\odot$ WD with 0.63 $M_\odot$ of ^{56}Ni and (2) the helium detonation sub–Chandrasekhar-mass WD model SC (Woosley & Weaver 1994b) for a 0.9 $M_\odot$ WD with 0.43 $M_\odot$ of ^{56}Ni. Model W7 is very similar in elemental composition and density profile of the core to other reasonable Chandrasekhar-mass models such as the delayed-detonation model DD4 (Woosley & Weaver 1994a). Significant difference exists in elemental composition and density profile between models W7 and SC. Model W7 predicts no ^{56}Ni within about 2000 km $\mathrm{s^{-1}}$ of the core center, which consists of mainly stable iron and nickel, while ^{56}Ni is present throughout the core for model SC. Model W7 predicts a higher density and a steeper density distribution than model SC, and the ratio of their densities ranges from about 5 in the core center to about 1 at the core edge at $v \approx 10^4\ \mathrm{km\ s^{-1}}$.

3. IONIZATION STRUCTURE

As the result of the different elemental compositions and density profiles, the ionization structures for models W7 and SC are drastically different in the inner region though similar in the outer region, as illustrated by the results at 300 days in Figure 1. For model W7, the ionization stage in the inner region within about 2000 km $\mathrm{s^{-1}}$ is much lower than that in the outer region. In the absence of ^{56}Co, the energy deposition in this inner region is entirely due to the γ-rays transported from the outer region, and it is much lower than that in the outer region, which is dominated by the positron kinetic energy deposition. The presence of the abundant neutral iron in the inner region excludes all the multiply charged ions in this region due to the rapid charge transfer between them. In the outer region, the presence of the abundant multiply charged ions effectively removes most of the neutral iron again because of the charge transfer between them. The ionization stage becomes higher as the velocity increases because the density decreases. For model SC, on the other hand, the overall ionization stage is higher because of the higher ^{56}Co fraction and lower density. The

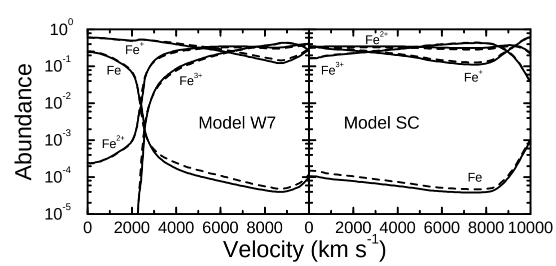

FIG. 1.—Calculated iron ionization structure of SNe Ia with (*solid lines*) and without (*dashed lines*) inclusion of the photoionization. Fractional abundances of neutral and ionized iron are shown as a function of the expansion velocity at 300 days since the supernova explosion for models W7 (*left*) and SC (*right*).

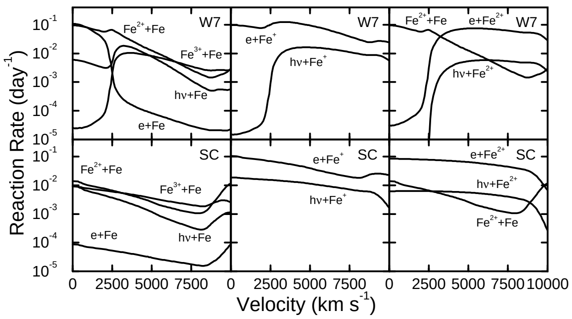

FIG. 2.—Reaction rates per particle for various important atomic processes are shown as a function of the expansion velocity at 300 days for models W7 (*upper panels*) and SC (*lower panels*) leading to the destruction of Fe (*left panels*), Fe^+ (*middle panels*), and Fe^{2+} (*right panels*).

singly and doubly charged ions dominate in the inner region, while the triply charged ions become abundant in the outer region where the density is lower. The neutral abundance is very small throughout the core as a result of the charge transfer.

As demonstrated in Figure 1, the difference introduced by including photoionization is small, with an increase of roughly 10% in the integrated mass ratio of Fe^{2+}/Fe^+. This is because the photoionization rates are much lower than the total rate of the fast electron impact ionization and charge transfer (Fig. 2). The ionization of neutral iron due to the charge transfer dominates its photoionization for both models W7 and SC (Fig. 2, *left*). For model W7, in the inner region where neutral Fe is abundant, the electron impact ionization of neutral Fe is as important as the charge transfer, and they are both much more important than the photoionization. The photoionization rate of Fe^+ is much lower than the electron impact ionization rate for both models, and the difference is particularly large for model W7 in the inner region where there are very few multiply charged ions (Fig. 2, *middle*). In the inner region, charge transfer becomes a dominant process in destroying Fe^{2+} for model W7, and in the outer region, the electron impact ionization rate dominates the photoionization rate by an order of magnitude (Fig. 2, *upper right*). For model SC, charge transfer and photoionization are both minor processes in destroying Fe^{2+} with the charge transfer dominating the photoionization in the inner and outer regions but with the photoionization dominating the charge transfer in the middle region (Fig. 2, *lower right*).

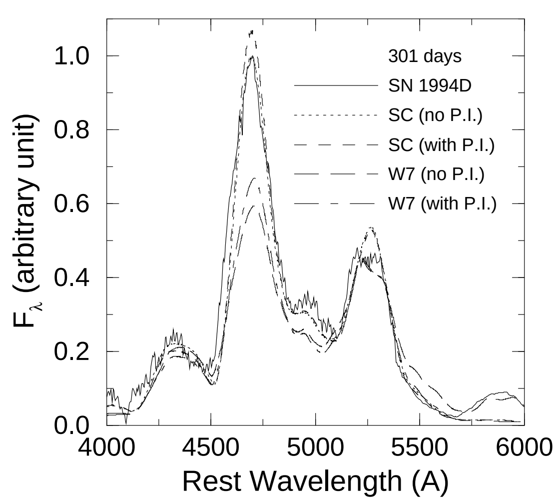

FIG. 3.—Comparison of the optical spectrum of SN 1994D at about 301 days with the synthetic spectra calculated assuming models W7 and SC with and without inclusion of photoionization.

Photoionization plays only a minor role in determining the ion abundances, largely because the recombination goes through a very complicated cascading process which substantially limits the efficiency of photoionization. The effect of the photoionization on the ion abundances is only roughly 10%, which is within the uncertainties of the atomic data for the other important atomic processes. On the other hand, because the recombination processes are efficient in producing photons that can ionize neutral Fe, the neutral abundance is affected significantly. However, photoionization of neutral Fe is less important than the combination of the electron impact and charge transfer. Depending on the region considered, this is either because the neutral abundance is so low that it is optically thin or because the presence of the abundant neutral Fe excludes the multiply charged ions in which the photons originate.

The relative importance of the charge transfer and photoionization depends critically on the input of atomic data, especially the fast electron impact ionization cross sections, recombination rate coefficients, and photoionization cross sections. For larger electron impact ionization cross sections, smaller recombination rate coefficients and larger photoionization cross sections, the neutral abundance would be smaller, the charge transfer rates would be smaller, and the photoionization rates would be larger. At times earlier than 300 days, the neutral photoionization is expected to be more significant because of the higher photoionization optical depth due to the higher density.

Our predicted iron ionization structure is qualitatively similar to but quantitatively different from that presented by Ruiz-Lapuente et al. (1995), who found a higher ionization stage for model W7 with high overall abundances of Fe^{2+} and Fe^{3+} of about 45% and 30%, respectively, and a low abundance of Fe^+ of no more than 20%. We obtained a generally lower ionization stage partly because we adopted the higher recombination rate coefficients calculated by Nahar (1996b, 1997) and Nahar et al. (1997), while the lower estimates of the rate coefficients by Woods et al. (1981) were used in the calculations of Ruiz-Lapuente et al. (1995). It is also because of our inclusion of the charge transfer, which reduces the abundances of the multiply charged ions and enhances the abundance of the singly charged ion. The difference may also be partly caused by the detailed difference between our Monte Carlo treatment of the energetic electron energy deposition (Liu & Victor 1994) and the approach of Ruiz-Lapuente et al. (1995) and by the different electron ionization cross sections that entered the two models. Our results should be more reliable because of the better quality of the atomic data used in our calculations and our more detailed treatment of the important atomic processes.

Although the relatively low neutral abundance makes any direct observable spectral signature of charge transfer unlikely, the charge transfer processes directly affect the abundances of the species and indirectly the synthetic spectra for SNe Ia. The change of the synthetic spectra due to the inclusion of the photoionization is small. In Figure 3, the normalized synthetic spectra for models W7 and SC with and without inclusion of the photoionization are compared with the 301 day optical spectrum of SN 1994D, a normal SN Ia. The spectral comparison with and without the inclusion of the photoionization have been presented in Liu et al. (1997a) and Liu et al. (1997c), respectively. It is evident that the Fe III feature at about 4700 Å will only be slightly stronger for both models W7 and SC if the photoionization is included and this change is within the uncertainty of the atomic data used in the spectral modeling. The synthetic spectra for model SC agree very well with the supernova spectrum, while those for model W7 are significantly different. The significant difference for model W7 will still remain even if the elemental composition of the core is mixed or ^{56}Ni only. Thus our previous conclusion is strengthened that the density profiles and elemental compositions of the iron core predicted by sub-Chandrasekhar-mass models are favored.

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