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FORMATION AND DESTRUCTION OF SILICON MONOXIDE IN SN 1987A

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ABSTRACT

We present a new chemistry model for the silicon monoxide molecules in SN 1987A. It incorporates an enhanced rate of formation by radiative association and an enhanced rate of destruction through charge transfer between SiO and Ar^+ and Ne^+ , which is more efficient than the energetic electron impact ionization and dissociation in a previous model. The conclusion is unchanged that the 10^{-4} – $10^{-3} M_{\odot}$ of SiO observed in SN 1987A can be produced by chemistry models in which there is no microscopic mixing of helium into the silicon-oxygen region of the ejecta.

Subject headings: molecular processes — supernovae: individual (SN 1987A)

1. INTRODUCTION

Infrared emission from vibrationally excited silicon monoxide molecules was observed in the ejecta of SN 1987A as early as 160 days after the supernova explosion (Aitken et al. 1988) and could no longer be detected after 578 days (Roche et al. 1989). The fundamental emission spectra of SiO have been analyzed by Liu & Dalgarno (1994). By accounting for optical depth effects on the emission and non-LTE effects on the vibrational level populations, Liu & Dalgarno (1994) have inferred 10^{-4} – $10^{-3} M_{\odot}$ for the mass of SiO in the ejecta.

The chemical processes that form and destroy SiO molecules in the supernova have been explored by Liu & Dalgarno (1994), who suggested that the radiative association of silicon atoms and oxygen atoms to form SiO is the major mechanism for the formation of SiO in the supernova. Liu & Dalgarno (1994) assumed a rate coefficient that is one order of magnitude smaller than the rate coefficient for the radiative association of carbon atoms and oxygen atoms to form CO (Dalgarno, Du, & You 1990). However, the rate coefficient for the radiative association to form SiO has now been calculated by Andreazza, Singh, & Sanzovo (1995). It is a factor of 30 larger than that adopted by Liu & Dalgarno (1994). Thus, more efficient destruction mechanisms for SiO must be operative in the supernova ejecta than the ionization and dissociation by energetic electron impact that were proposed by Liu & Dalgarno (1994).

We point out in this paper chemical reactions that destroy SiO in the ejecta that can balance the more rapid formation of SiO. The presence of argon and neon in the silicon-oxygen region of the ejecta significantly enhances the efficiency of destruction of SiO in the supernova due to charge transfer reactions with Ar^+ and Ne^+ . As a result, the conclusion of our earlier chemistry model (Liu & Dalgarno 1994) remains valid that the 10^{-4} – $10^{-3} M_{\odot}$ of SiO observed in SN 1987A can be produced by chemistry models in which there is no microscopic mixing of helium into the silicon-oxygen region of the supernova ejecta.

2. CHEMISTRY OF SiO

We have explored the chemical processes that form and destroy silicon monoxide molecules in SN 1987A, in addition to those presented in our previous model (Liu & Dalgarno 1994). The SiO chemistry depends on the elemental composition of the silicon-oxygen region of the supernova ejecta and the degree of mixing of other elements in this

region. Dynamical instabilities during and after the supernova explosion cause macroscopic mixing of elements in different layers rather than microscopic mixing. We used unmixed models with the elemental compositions predicted by the explosive nucleosynthesis models of Woosley, Pinto, & Weaver (1988) and of Thielemann, Hashimoto, & Nomoto (1990). For the composition of Woosley et al. (1988), $0.14 M_{\odot}$ of silicon and $0.02 M_{\odot}$ of oxygen in the silicon-oxygen region are mixed with $0.06 M_{\odot}$ of sulfur, $0.0093 M_{\odot}$ of argon, and $0.0043 M_{\odot}$ of calcium. The adjacent region, which contains most of the oxygen mass in the supernova, is not expected to be a major site for SiO formation because neon is the dominant constituent in this region and Ne^+ is effective in destroying the SiO molecules even if there is silicon mixed into the region. For the composition of Thielemann et al. (1990), SiO is likely to be abundant in the region where there is $0.01 M_{\odot}$ of silicon and $0.1 M_{\odot}$ of oxygen together with $0.004 M_{\odot}$ of sulfur, $0.007 M_{\odot}$ of magnesium, and a small amount of carbon. In other regions with significant amounts of silicon, SiO is not expected to be abundant, either because of the deficiency of oxygen or because of destruction by Ne^+ and Ar^+ . To investigate the sensitivity of the chemistry to possible microscopic mixing, we also used the composition in the mixed model of Nomoto et al. (1991) in which $0.085 M_{\odot}$ of silicon and $1.48 M_{\odot}$ of oxygen are mixed with $0.114 M_{\odot}$ of carbon, $0.147 M_{\odot}$ of magnesium, $0.229 M_{\odot}$ of neon, $0.0229 M_{\odot}$ of sulfur, $0.00378 M_{\odot}$ of argon, $0.00325 M_{\odot}$ of calcium, $0.073 M_{\odot}$ of iron, and other minor elements.

The chemistry is not sensitive to the temperature, and we assumed that the gas kinetic temperature is the same as the temperature derived by Liu & Dalgarno (1994) from the rotational level populations of SiO, which is about 2000 K. We assumed that the silicon-oxygen region of the ejecta expanded homologously with the density

$$n = 7 \times 10^{10}(t/100 \text{ days})^{-3} \text{ cm}^{-3}, \quad (1)$$

at time t after the supernova explosion (Liu & Dalgarno 1994).

2.1. Formation of SiO

There was no evidence of dust formation in the ejecta of SN 1987A until about 530 days after the supernova explosion (Lucy et al. 1991). In the absence of grains, molecular formation in the gas phase must have been initiated by radiative processes. Liu & Dalgarno (1994) suggested that

the direct radiative association

is the most important mechanism for the formation of SiO molecules in SN 1987A. Its rate coefficient has been calculated by Andreazza et al. (1995) to be $5.52 \times 10^{-18} T^{0.31 \pm 0.02} \text{ cm}^3 \text{ s}^{-1}$, where T is the temperature in degrees kelvin. The formation of SiO may also be accomplished indirectly by the radiative association

with a rate coefficient of $9.7 \times 10^{-19} - 7.4 \times 10^{-23} T + 4.4 \times 10^{-27} T^2 \text{ cm}^3 \text{ s}^{-1}$ (Andreazza et al. 1995), followed by charge transfer reactions with metals such as

However, this sequence is an unimportant source of SiO because SiO^+ is destroyed predominantly by dissociation recombination

Dissociation recombination proceeds rapidly in the supernova ejecta, which has an ionization fraction of 10^{-2} . An additional source of SiO is provided by the radiative association

with a rate coefficient of about $8.5 \times 10^{-21} \text{ cm}^3 \text{ s}^{-1}$ at 2000 K (Babb & Dalgarno 1995), followed by the neutral reaction

with a rate coefficient of $2.7 \times 10^{-10} \text{ cm}^3 \text{ s}^{-1}$ (Husain & Norris 1978) or $9 \times 10^{-12} \text{ cm}^3 \text{ s}^{-1}$ (Swearengen, Davies, & Niemczyk 1978). The sequence initiated by radiative attachment

followed by associative detachment

is a negligible path for the formation of SiO molecules in the ejecta because the negative ions are effectively destroyed by photodetachment

and by mutual neutralization such as

2.2. Destruction of SiO

2.2.1. Energetic Electron Impact

The silicon monoxide molecules formed in SN 1987A can be destroyed by impacts with energetic electrons created by

the decay of the radioactive nuclei ^{56}Co and ^{57}Co . The fast electrons can ionize and dissociate SiO,

(Liu & Dalgarno 1994). The similar processes for carbon monoxide have been analyzed in detail (Liu & Victor 1994) and applied to the CO chemistry of SN 1987A (Liu, Dalgarno, & Lepp 1992; Liu & Dalgarno 1995). We assumed the same rate of destruction by energetic electron impact for SiO as for CO. For an average energy deposition rate per particle in the oxygen core of

$$L = 60 \exp(-t/\tau) \{1 - \exp[-\phi_0(t/t_0)^{-2}]\} \text{ eV day}^{-1}, \quad (21)$$

where $\tau = 111.26$ days and $\phi_0 = 31.1$ at $t_0 = 100$ days (Liu & Dalgarno 1995), and for a mean energy per ion pair of about 30 eV for SiO, the rate of destruction of SiO by energetic electron impact can be estimated to be

$$R = 2 \exp(-t/\tau) \{1 - \exp[-\phi_0(t/t_0)^{-2}]\} \text{ day}^{-1}. \quad (22)$$

Since the radiative association (2) proceeds faster than assumed in our previous chemistry model (Liu & Dalgarno 1994) in which energetic electron impact is the dominant mechanism for the destruction of SiO in SN 1987A, more efficient destruction mechanisms must exist and will be explored below.

2.2.2. Photodissociation and Photoionization

A possible mechanism for the destruction of SiO in SN 1987A is provided by photodissociation and photoionization. The ultraviolet photons are produced by excitation of atoms and ions by energetic electron impact and by recombination of ions following ionization by energetic electron impact. These energetic electrons are produced following radioactive decay of ^{56}Co and ^{57}Co . An estimate of the ultraviolet flux of $4 \times 10^{15} \text{ photons cm}^{-2} \text{ s}^{-1}$ was made by Petuchowski et al. (1989), based on the tentative identification by Moseley et al. (1989) of a spectral feature at $22.9 \mu\text{m}$ as an emission line of Fe^{2+} . Petuchowski et al. (1989) assumed that the relative abundance of $\text{Fe}^{2+}/\text{Fe}^+$ is controlled by a balance between the photoionization of Fe^+ and the charge transfer of Fe^{2+} with neutral oxygen. About half of the photons ionizing Fe^+ are energetic enough to destroy SiO.

Even if the identification of the Fe^{2+} emission line is accepted, no other doubly charged species having been found in the ejecta, the inferred ultraviolet flux is too large because the analysis ignores the ionization caused by energetic electrons. Li, McCray, & Sunyaev (1993) have shown that the observed infrared emission of Fe^+ can be accounted for by fast electrons for the first two years, with the ultraviolet photons contributing only at later times. Because the core experienced a considerable expansion driven by the large deposition of energy (Li et al. 1993), the density is low. There is little oxygen or elements other than iron, and Fe^{2+} is removed slowly by radiative and dielectronic recombination and by charge transfer

to the neutral iron component.

Considerable shielding of any ultraviolet flux by neutral silicon and by SiO itself is also to be expected so that only the chemistry on the surface of the clumps containing the Si and the O will be affected. The optical depth of the silicon contained in a velocity interval as small as 1 km s^{-1} is of the order of 10^5 for a photoionization cross section of 10^{-17} cm^2 (Conneely, Smith, & Lipsky 1970; Chapman & Henry 1972). The mean photodissociation cross section of SiO is probably of the order of 10^{-18} cm^2 so that even with high flux (Petuchowski et al. 1989) the unshielded dissociation rate is only 10^2 day^{-1} and the shielded rate is 10^{-3} day^{-1} , much lower than the destruction rate due to energetic electron impact.

2.2.3. Charge Transfer

In the absence of microscopic mixing of helium in the silicon-oxygen region of the ejecta, the dissociative charge transfer reactions

do not occur. The reactions

are unimportant mechanisms for destruction of the SiO molecules in the supernova even if the carbon comingles with the SiO because rapid charge transfers to metals such as

cause the carbon to be mostly neutral in the ejecta. An important mechanism for the destruction of the SiO molecules in SN 1987A is provided by the charge transfer reactions

Silicon and argon together with sulfur and calcium are the main products of oxygen burning during the explosive nucleosynthesis, and they are intermixed together in the supernova ejecta. Neon is produced in the stellar nucleosynthesis during the main sequence, and neon and oxygen are mixed microscopically in the supernova ejecta. The substantial presence of argon and neon in the silicon-oxygen region significantly enhances the destruction efficiency for the SiO molecules in SN 1987A. Reactions (31)–(33) should proceed more rapidly than the corresponding reactions of CO:

because SiO is less stable than CO. The rate coefficient for reaction (34) has been measured to be about $4 \times 10^{-11} \text{ cm}^3 \text{ s}^{-1}$ at the center-of-mass kinetic energy of 0.1 eV (Rebrion, Rowe, & Marquette 1989; Flesch, Nourbakhsh, & Ng

1991). Reaction (35) proceeds at a rate coefficient of $2 \times 10^{-12} \text{ cm}^3 \text{ s}^{-1}$ at 0.2 eV, and the rate coefficient increases rapidly as the kinetic energy increases (Jones et al. 1981; Villinger et al. 1983). We assumed rate coefficients of $4 \times 10^{-11} \text{ cm}^3 \text{ s}^{-1}$ and $2 \times 10^{-12} \text{ cm}^3 \text{ s}^{-1}$ for reactions (31) and (32)–(33), respectively.

The efficiency of Ar^+ and Ne^+ in destroying SiO depends directly on the ionization fractions of argon and neon in the silicon-oxygen region of the supernova ejecta, which are controlled by charge transfer reactions of Ar^+ and Ne^+ with neutral atoms. Charge transfer reactions involving noble ions are likely to be slow. The charge transfer reaction

proceeds slowly, with a rate coefficient of $5.2 \times 10^{-14} \text{ cm}^3 \text{ s}^{-1}$ at 2000 K (Kimura et al. 1993). The rate coefficient for the charge transfer reaction,

is negligibly small (Kimura et al. 1994). We assumed that charge transfer reactions such as

are slow, with rate coefficients in the range around $10^{-13} \text{ cm}^3 \text{ s}^{-1}$ so that the ionization fractions of argon and neon are high, and we assumed that charge transfer reactions such as

are rapid with rate coefficients of $10^{-9} \text{ cm}^3 \text{ s}^{-1}$.

3. MASS OF SiO IN SN 1987A

Shown in Figure 1 and listed in Table 1 are the masses of SiO in SN 1987A derived from the fundamental emission spectra of SiO by taking into account optical depth effects

FIG. 1.—The SiO mass in SN 1987A as a function of time since the supernova explosion. The closed circles are the observed masses derived by Liu & Dalgarno (1994) from the fundamental emission spectra of SiO by taking into account the optical depth effects and departures from local thermodynamic equilibrium. The solid, dashed, and dot-dashed lines are the predictions of the chemistry for the elemental compositions of Woosley et al. (1988), Thielemann et al. (1990), and Nomoto et al. (1991), respectively.

TABLE 1
MASS OF SiO IN SN 1987A

EPOCH (days)	OBSERVED MASS	PREDICTED MASS FROM CHEMISTRY		
	Liu & Dalgarno (10^{-4})	Woosley et al. ($10^{-4} M_{\odot}$)	Thielemann et al. ($10^{-4} M_{\odot}$)	Nomoto et al. ($10^{-4} M_{\odot}$)
257.....	3.4	4.4	11.9	8.4
260.....	4.4	4.4	11.8	8.3
279.....	4.5	4.2	11.4	7.9
290.....	5.7	4.1	11.2	7.8
313.....	6.0	4.1	11.1	7.7
370.....	5.8	4.5	11.7	8.3
400.....	6.4	5.0	12.4	9.0
404.....	7.4	5.1	12.6	9.1
408.....	6.4	5.2	12.7	9.2
415.....	6.5	5.3	12.9	9.5
463.....	9.3	6.9	14.9	11.5
465.....	6.9	7.0	15.0	14.6
517.....	7.1	9.7	17.8	14.8
517.....	8.6	9.7	17.8	14.8
519.....	8.0	9.9	18.0	15.0

and departures from local thermodynamic equilibrium (Liu & Dalgarno 1994). The observed SiO masses increase significantly from 257 days to 465 days, followed by a slight decrease to 519 days. The absence of SiO emission after 530 days (Lucy et al. 1991) indicates that the SiO molecules were depleted into dust grains for which the SiO molecules themselves may have provided the seed.

These observed masses of SiO are in good agreement with the masses of SiO predicted for the various supernova models that are shown in Figure 1 and listed in Table 1. Similar to the temporal behavior of the observed SiO masses, the predicted SiO masses increase significantly after about 300 days. They depend on the elemental composition. The observed SiO masses are best reproduced by the chemistry model based on the composition of Woosley et al. (1988), for which the observed and predicted SiO masses agree within a factor of 1.5. The SiO masses predicted by the chemistry models with the compositions of Thielemann et al. (1990) and Nomoto et al. (1991) overestimate the observed SiO masses by factors of no more than 3.5. Thus, the chemistry is robust and not very sensitive to the elemental composition.

The predicted minimum SiO mass of $4 \times 10^{-4} M_{\odot}$ at about 300 days for the composition of Woosley et al. (1988) is lower by a factor of about 2 than the previous estimate of $7 \times 10^{-4} M_{\odot}$ (Liu & Dalgarno 1994). The SiO is formed mainly by the radiative association (2) and is destroyed mainly by the charge transfer reaction (31) with Ar^+ . Although the rate coefficient of the radiative association (2) is about 30 times higher than assumed in our previous model, the SiO formation rate is enhanced by an effective factor of only about 4 because the oxygen mass in the SiO-forming region is only $\frac{1}{7}$ of the total oxygen mass in the

supernova, most of it being in the region in which neon is the dominant element and the charge transfer reactions (32)–(33) limit the abundance of SiO. The presence of argon enhances the SiO destruction rate by a factor of about 7 through the charge transfer reaction (31). The significant increase at late times in the predicted SiO mass occurs because the destruction of SiO by Ar^+ becomes slower as the result of the rapid decrease in the fractional abundance of Ar^+ . The loss of Ar^+ is dominated at early times by the charge transfer reactions (38)–(39), with Si and O and accelerated at late times by the charge transfer reaction (31) with SiO as the fractional abundance of SiO increases.

For the compositions of Thielemann et al. (1990) and Nomoto et al. (1991), the chemistry models predict about $1 \times 10^{-3} M_{\odot}$ and $8 \times 10^{-4} M_{\odot}$, respectively, for the SiO masses at 300 days.

The predicted SiO masses would be reduced by orders of magnitude were the SiO molecules mixed microscopically with helium because the destruction of SiO by the dissociative charge transfer reactions (24)–(25) is extremely fast. Thus, the SiO chemistry permits no microscopic mixing of helium in the silicon-oxygen region where SiO is abundant.

These additional destruction mechanisms for SiO in SN 1987A through the charge transfer reactions (31)–(33) have no effect on the chemistry of CO (Liu et al. 1992; Liu & Dalgarno 1995) because the argon and neon do not mix into the carbon-oxygen region of the supernova ejecta where the CO molecules are formed.

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