Molecules and dust in the early universe: the supernova connection

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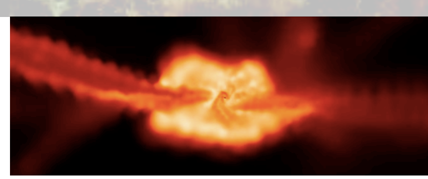

The First Stars and Galaxies: Challenges for the Next Decade

March 8-11, 2010

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Overview

- Evidence for dust in supernovae
- Chemical kinetics versus other dust synthesis formalisms
- What kind of dust ? Chemical routes
- Models for primitive supernovae
- Molecules and dust in PISNe
- Depletion efficiencies and mixing
- Conclusions

Evidence for molecules and dust in Supernovae

Dust in nearby Type IIp supernovae:

- SN1987A : IR detection of **CO, SiO** and dust (from ~ **350 days** to ~ **800 days** post-explosion) - **10^{-4} - 10^{-3} M_{sun}** (Roche et al. 1991, Meikle et al. 1993, Ercolano et al. 2007)
- SN2003gd: dust observed with Spitzer - **10^{-2} M_{sun}** (Sugerman et al. 2006)
- No large amounts of dust detected in SN2004dj - **4 10^{-5} M_{sun}** (Meikle et al. 2007), or SN2004et **~ 10^{-4} M_{sun}** (Kotak et al. 2009) – detection of **CO and SiO**.
- Dust amounts observed in SNRs: Cas A ~ **0.1 M_{sun}** in IR+Submm
- From isotopic anomaly analysis of meteoritic grains: stardust inclusions formed in Type II SN ejecta – graphite, silicates, SiC, and Si_3N_4 (Zinner 2006)

-Are local CCSNe efficient dust makers? $1e^{-1}$-$1e^{-6}$ M_{sun}

-Silicate, metal oxide and/or carbon grains or a mixture?

At high redshift (< 1Gyr or z > 6)

- Large amount of dust deduced from reddening of background quasars: **J1148+5251 at z = 6.4: M_{dust} = (0.9 - 4) 10^8 M_{sun}** - M_{dust}/M_{gas} = 0.5 -1 10^{-2}
- Dust mass implies a **dust yield of ~ 1 M_{sun}/SN** (Dwek et al. 2007).
- Difficult to reconcile with local CCSNe.

Chemical kinetics versus other formalisms

- **Thermodynamic equilibrium** used in meteorite studies (Fedkin et al. 2010):
  P-T phase diagram inappropriate for dynamical outflows out of equilibrium.
- **Classical nucleation theory**: dust formation in SNe and AGB stars
(Draine 1979, Kozasa et al. 1989, Todini & Ferrara 2001, Nozawa et al. 2003, Schneider et al. 2004, Ferrarotti & Gail 2006)

involves concepts like **surface tension**, **sticking coefficient**, **supersaturation ratio, equilibrium distribution of critical clusters…**
can't apply to Å size dust precursors out of equilibrium (Donn & Nuth 1985)

… Ignore the chemical synthesis of molecules and dust precursors from the gas phase…

Chemical kinetic approach:

Nucleation of gas phase dust precursors + condensation (coagulation+surface growth)

Couple **the gas phase** to **the solid phase**

Very **general** and **powerful** approach which can be applied to any **stellar outflow…**

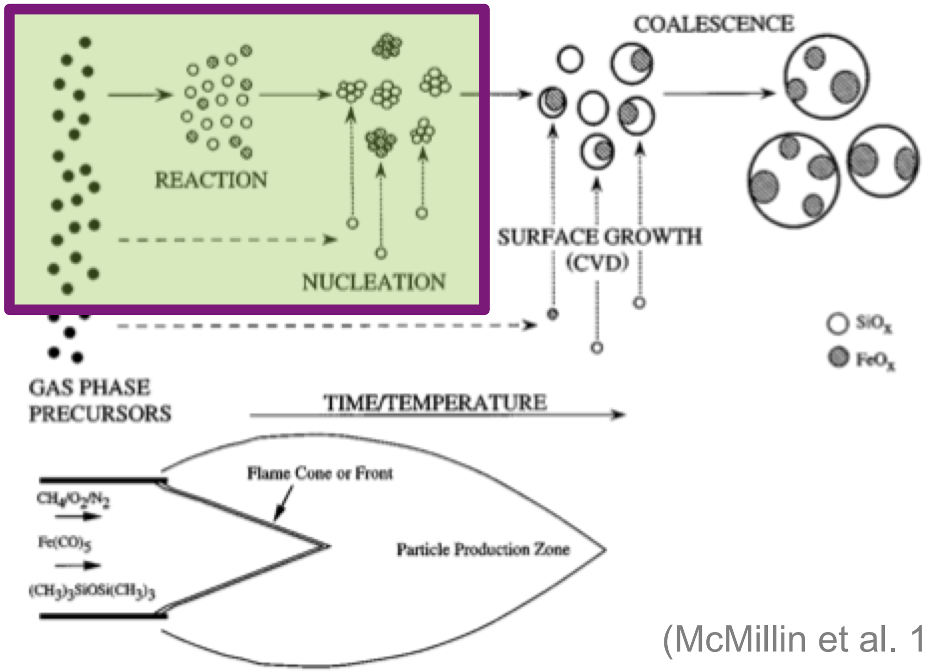
Chemical kinetics versus other formalisms

In the laboratory, we can form dust from the gas phase using different techniques:

- Vaporization of solid rods
- Pyrolysis of hydrocabons
- Flame aerosol reactors

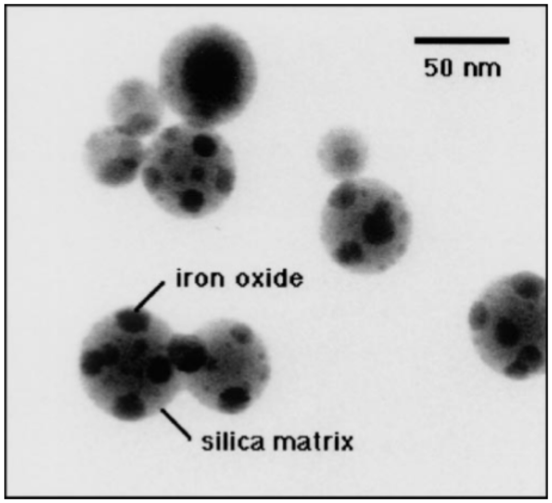
Study the synthesis of **soot, metal oxides, silicate, metal carbide dust**…

(Kaito et al. 2003, Jäger et al. 2009)

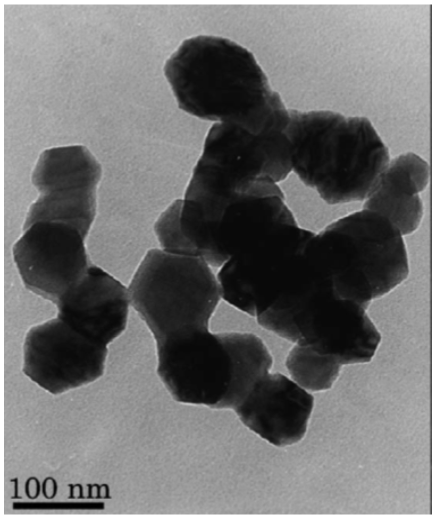


(McMillin et al. 1996)

Fe_2SiO_4 - Fayalite



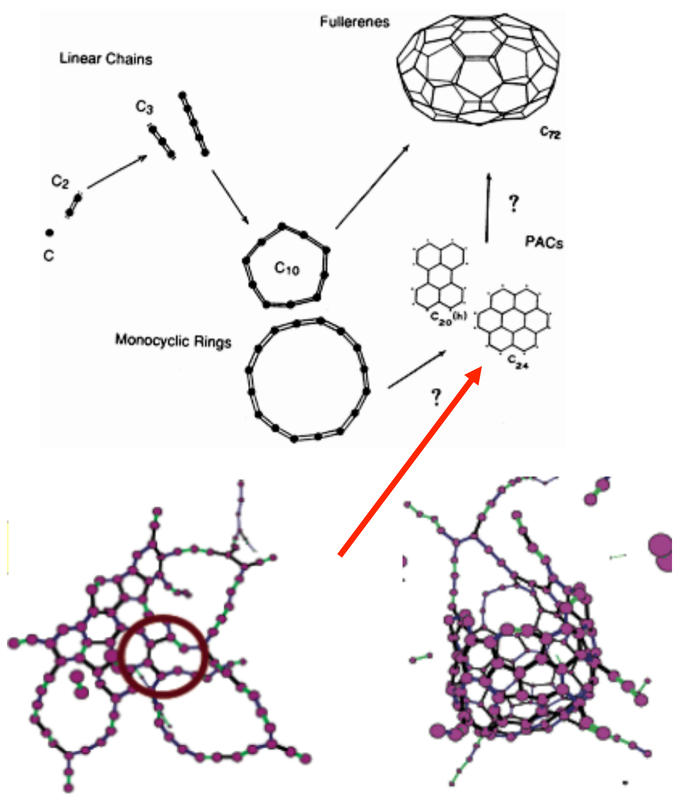
FeS - Troilite



What kind of dust? Some chemical routes

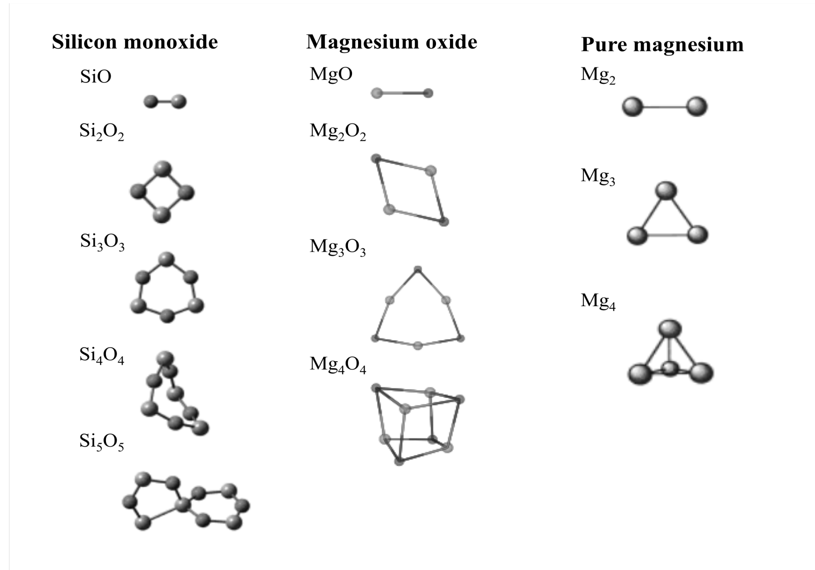
Amorphous carbon:

Without hydrogen: carbon chains & rings



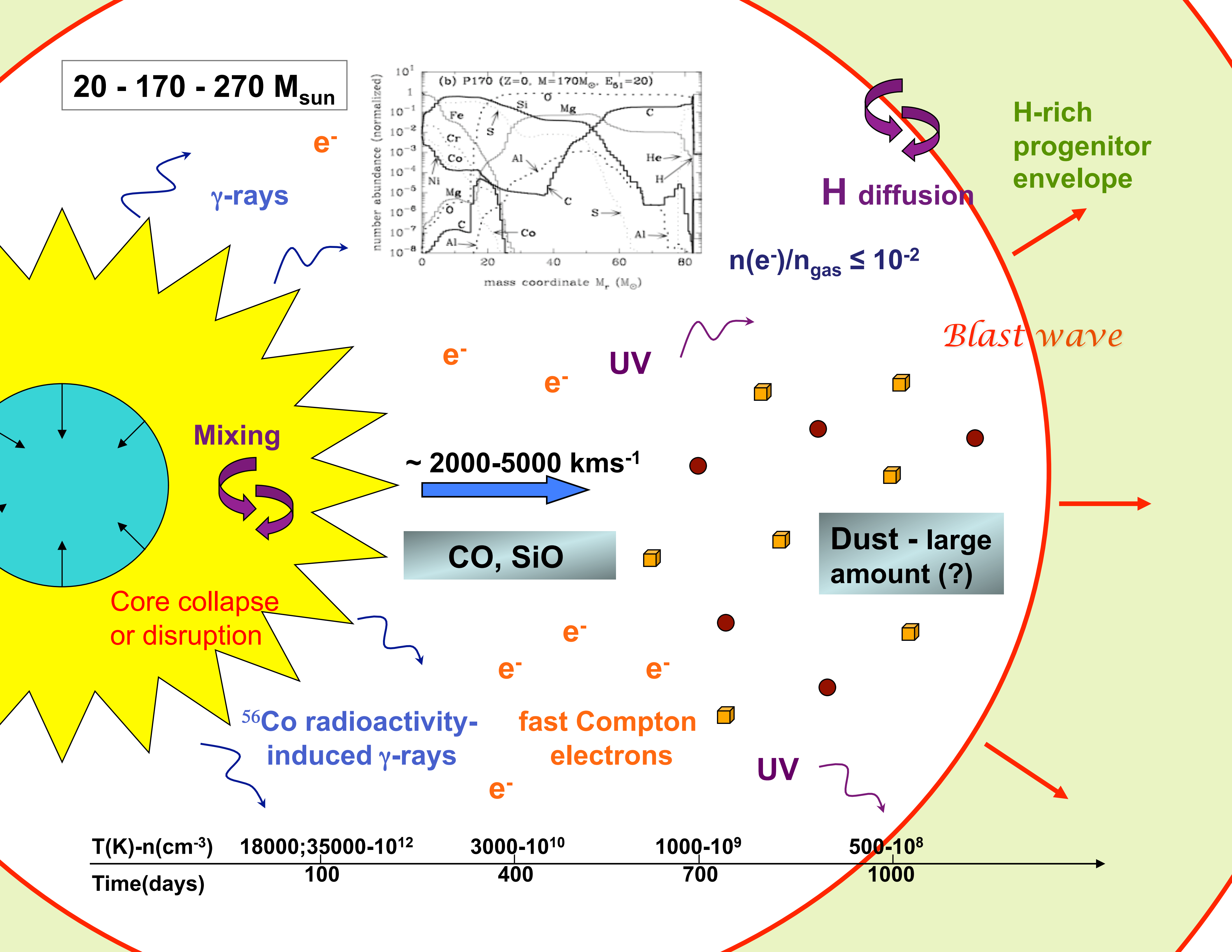
(Cherchneff et al. 2000, Irle et al. 2003)

Silica, metals and oxides



- Slow radiative association reactions for **carbon chains** formation from **free C** (Clayton et al. 1999, 2001)
- Pressure dependent nucleation rate for silica (Zachariah & Tsang 1993)
- Not all chemical steps and intermediates are characterized ⟶ rely on experiments (kinetics & intermediate identification) and theory (structure, TS)

No a priori assumption on what kind of dust forms
All chemical routes apply to AGBs, Supergiants, Wolf-Rayet CWR, R CrB stars, or SN ejecta



20 - 170 - 270 M$_{sun}$
(b) P170 (Z=0, M=170M$_\odot$, E$_{51}$=20)
number abundance (normalized)
mass coordinate M$_r$ (M$_\odot$)
H diffusion
H-rich progenitor envelope
γ-rays
e-
n(e-)/n$_{gas}$ ≤ 10^{-2}
Blast wave
UV
Mixing
~ 2000-5000 kms^{-1}
CO, SiO
Dust - large amount (?)
Core collapse or disruption
^{56}Co radioactivity-induced γ-rays
fast Compton electrons
T(K)-n(cm^{-3})
18000;35000-10^{12}
3000-10^{10}
1000-10^{9}
500-10^{8}
Time(days)
100
400
700
1000

Primitive PISN and CCSN models

Chemical kinetic network: ~ 80 species and ~ 500 reactions with measured/theoretical rates from **astrochemistry**, **aerosol** and **combustion chemistry**, and **material science.**

Formation processes

- Tri- and bi-molecular reactions (neutral-neutral and ion-molecules),
- Radiative associations (e.g., carbon chains)

Destruction processes

- Radioactivity-induced Compton e^- destruction (dissociation, ionization),
- Thermal fragmentation (high T),
- UV photodissociation and ionization,
- Dissociative recombination of ions and ion attack (O^+, He^+)

Species **Linear, chains, rings** from H, O, C, N, Si, S, He, Al, Mg, and Fe.

- CO, SiO, SO, CO_2, SiS, SiO_2 O_2, ions (CO^+, SiO^+, and all metals)
- $(FeO)_n$, $(MgO)_n$,,$(SiO)_n$, $(SiO_2)_n$, AlO, $(Mg)_n$, $(Fe)_n$, $(Si)_n$, $(FeS)_n$, $(MgS)_n$; n=1-4
- Carbon chains [C_2 – C_9] and ring C_{10}

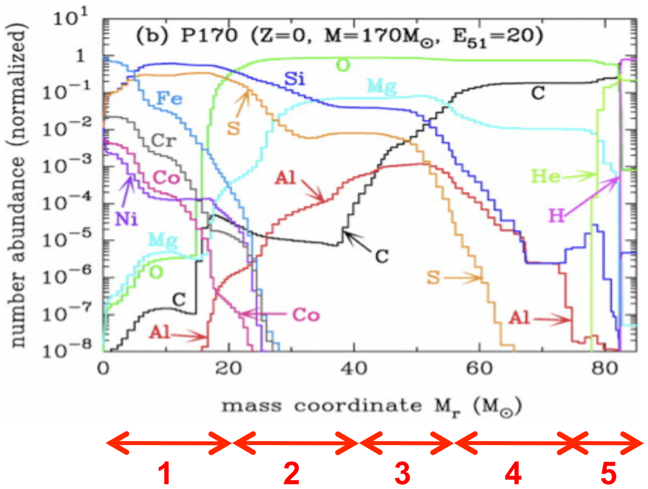
Two ejecta mixing extreme cases:

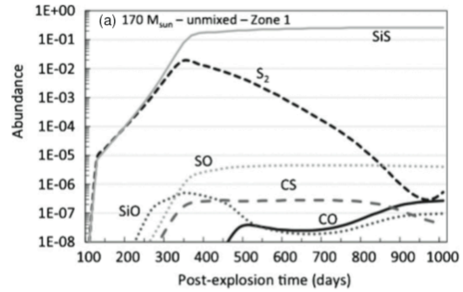
- **fully microscopically mixed He core** (Umeda & Nomoto 2002, Heger & Woosley 2002),
- **stratified He core where each zone is microscopically mixed** (Nozawa et al. (2003),

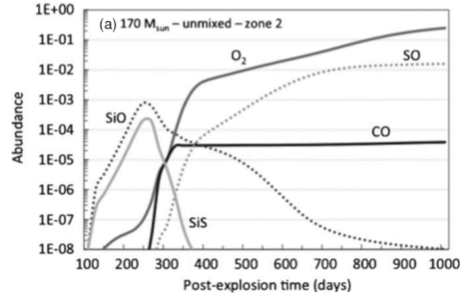
- **Temperature and density** profiles from Nozawa et al. (2003).
- **Velocity** : v = 2000- 5500 kms^{-1}.

Results: molecules and dust clusters in PISNe

1 - 170 Msun unmixed







- Chemistry **is not** at **steady- state**
- A 170 M_{sun} ejecta forms ~ **35 M_{sun}** of molecules at day 1000:

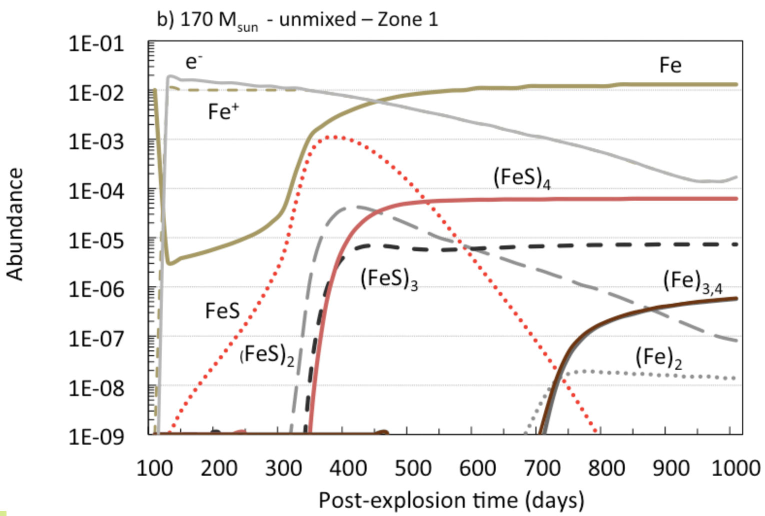
O_2 ($15M_{sun}$),

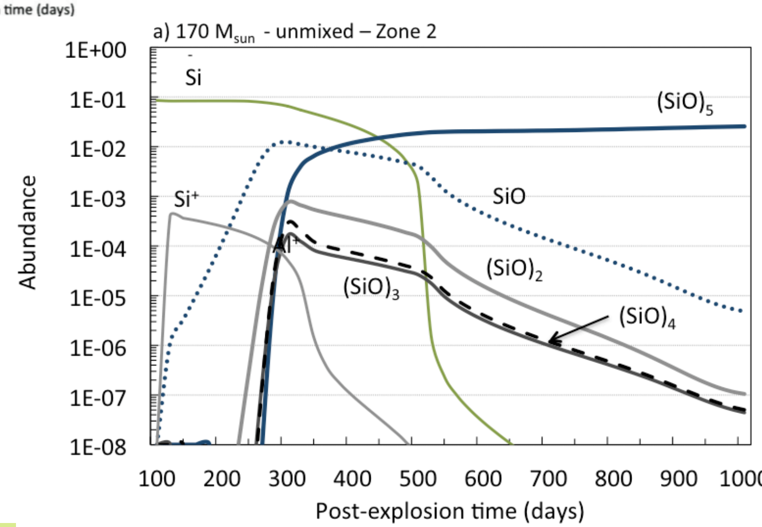
CO ($11M_{sun}$),

SiS ($8M_{sun}$),

SO ($1M_{sun}$).

(Cherchneff & Lilly 2008, Cherchneff & Dwek 2009)



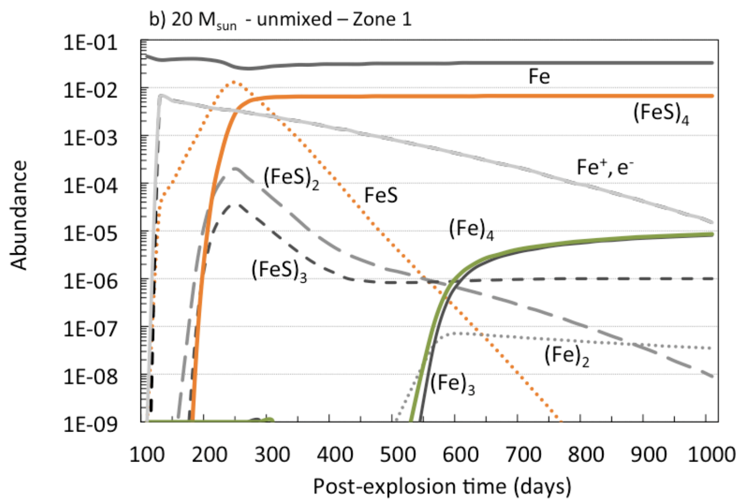


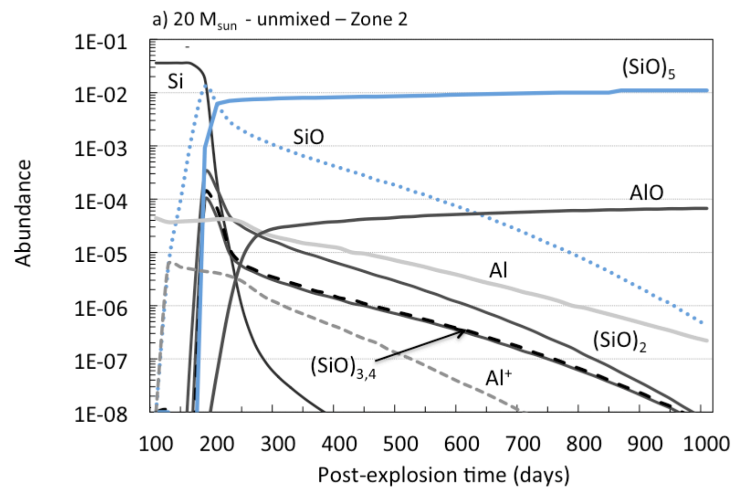
Cherchneff & Dwek (2010)

- **~ 6 M_{sun} of Silica (SiO_2)/silicate (forsterite Mg_2SiO_4), pure Si dust (99.5%), troilite (FeS) and alumina (Al_2O_3) (0.5%) is ejected at 1000 days equivalent to 3.5 % of progenitor mass,**
- **no carbon dust forms in Zones 4 & 5 due to oxidation of chains by O and dissociation by He^+ attack.**

Results: molecules and dust clusters in PISNe

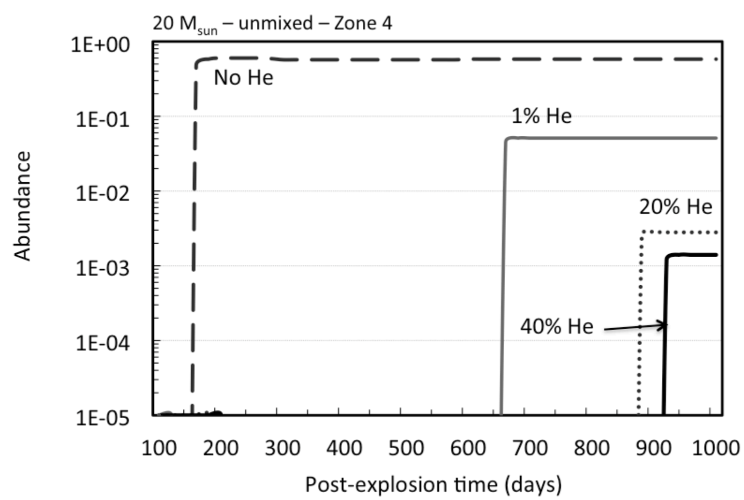
1 - 20 Msun unmixed





Cherchneff & Dwek (2010)

Zone 4: **He-rich; C/O ~ 26**

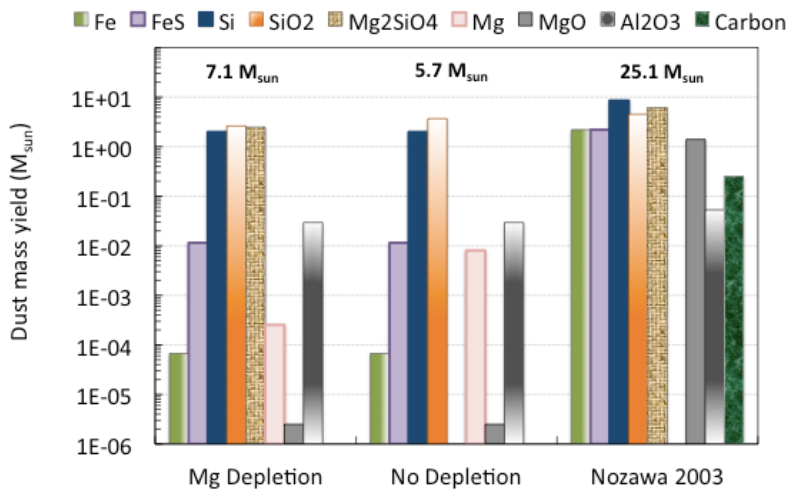


C_{10} abundance

Carbon ring C_{10} forms in Zones 4 (C/O>1) if He^+ absent (~0.014 M_{sun})

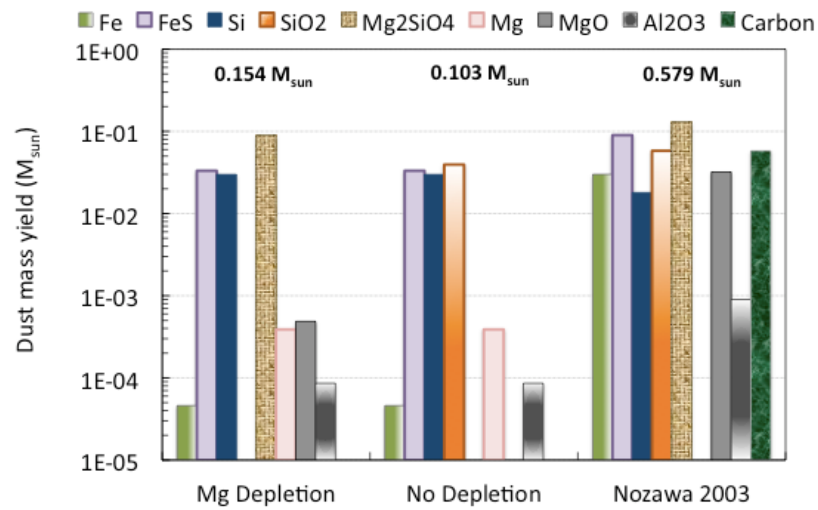
Results: molecules and dust precursors

170 M_{sun} progenitor unmixed ejecta



(Cherchneff & Dwek 2010)

20 M_{sun} progenitor unmixed ejecta



	Molecules (M_{sun})	Dust (M_{sun}) Depletion	Dust (M_{sun}) No depletion
Unmixed 170 M_{sun}	**35**	**7.1**	**5.7**
% of prog. Mass	**20.6%**	**4.2%**	**3.3%**
Unmixed 20 M_{sun}	**1.5**	**0.154**	**0.103**
% of prog. Mass	**7.5%**	**0.8%**	**0.5%**

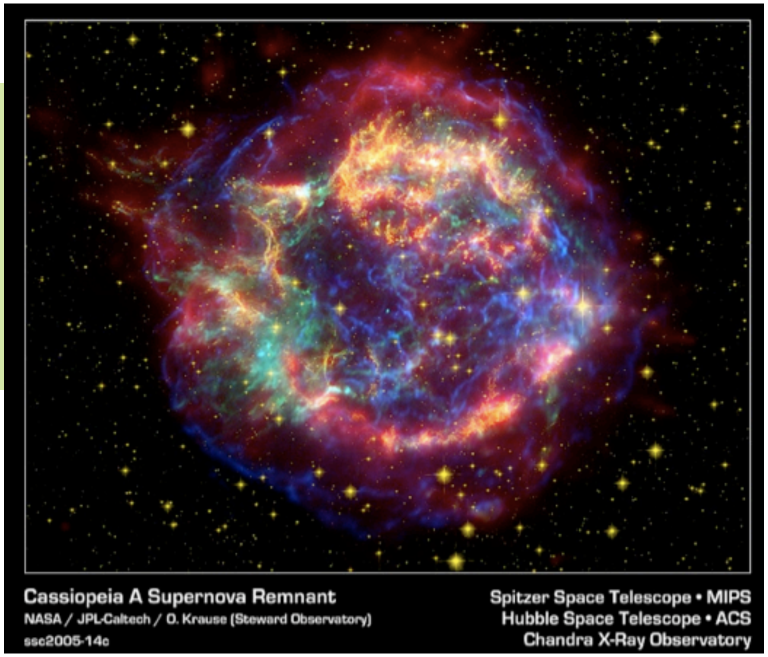
Existing models:

Nozawa et al. 2003: ***for a PISN, M_{dust}/M_{prog}* ~ 15 - 30% - for *20 M_{sun} CCSN*, M_{dust}/M_{prog} ~ 3 – 4%**

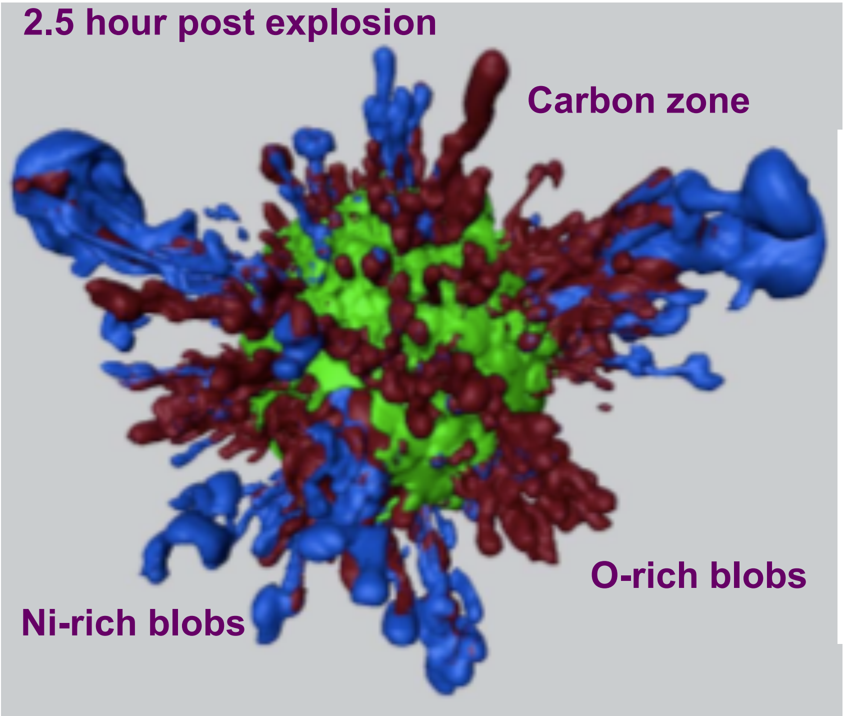
- **Our dust upper limits are smaller by a factor ~5 than dust budgets from existing models**
- **Dust clusters imply a different dust chemical composition**
- **Chemistry and molecular formation act as a bottleneck to dust formation**

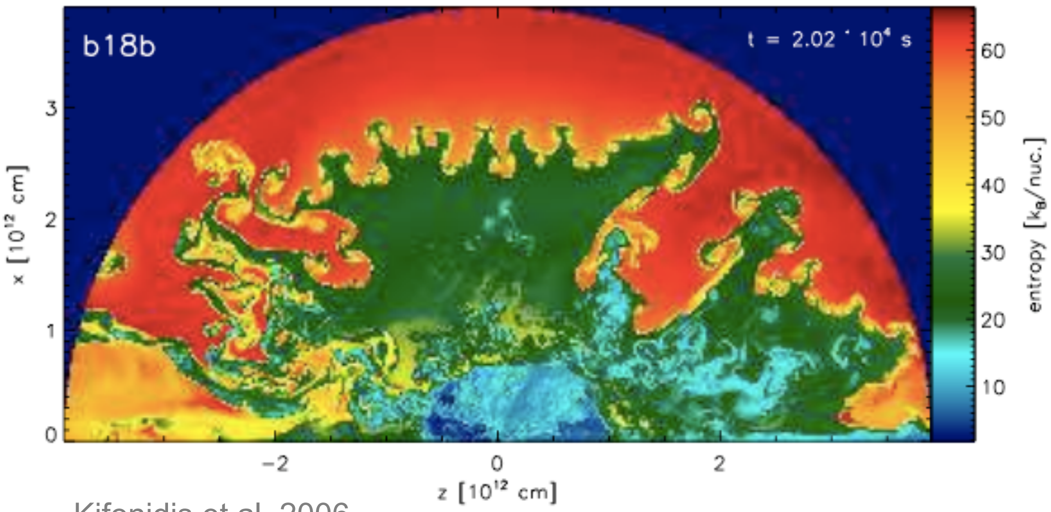
Depletion efficiencies and mixing

- Observational/theoretical evidence for mixing in local SNe and SN remnants
- Evidence **for microscopic mixing of non-adjacent layers from SiC and Si_3N_4** inclusions in meteorites



(Hammer et al. 2009)





Kifonidis et al. 2006

Depletion efficiencies and mixing

Depletion Efficiencies of Metals in Molecular Clusters and Molecules (Underlined) for the 170 and 20 $M_\odot$ Unmixed Ejecta[a]

		170 $M_\odot$					20 $M_\odot$			
Element	Clusters	Zone 1	Zone 2	Zone 3	Zone 4	Zone 5	Zone 1	Zone 2	Zone 3	Zone 4
Si	$(SiO_2)_5$	...	50.0%	50.0%	46.7%	37.2%	0.12%	49.5%	48.2%	...
	$(Si)_{4.5}$	1.8%	50.0%	50.0%	46.7%	37.2%	3.1%	49.5%	48.2%	...
	SiS	26.5%	...	...	...	...	28.3%	...	...	...
O	$(SiO_2)_5$	...	9.6%	2.7%	...	...	...	3.9%	...	...
	O_2	...	38.0%	46.4%	12.3%	...	...	60.9%	27.6%	...
	CO	...	...	...	29.1%	43.0%	...	...	32.7%	...
	SO	...	1.2%	0.3%	0.1%	...	0.7%	...	...	...
S	$(FeS)_4$	0.09%	...	...	...	...	8.7%	...	...	...
	SiS	98.9%	...	...	...	...	91.4%	...	...	...
	SO	...	100%	99.8%	...	...	...	99.2%	...	...
Al	AlO	...	97.0%	98.3%	92.1%	...	...	99.1%	96.8%	...
Fe	$(FeS)_4$	1.8%	...	...	...	...	44.0%	...	...	...
	$(Fe)_4$	0.02%	...	...	...	...	0.1%	...	...	...
Mg	$(Mg)_4$	...	0.1%	2.3%	0.1%	...	...	0.91%	0.04%	...
	$(MgO)_4$	...	...	...	...	...	...	...	0.73%	...
C	C_{10}	...	...	...	...	0%–21.6%[b]	...	...	...	0%–95.3%[b]
	CO	...	...	100.0%	100.0%	77.3%	...	99.8%	99.7%	0%–0.14%[b]

- Si is **totally depleted** by silica/silicate dust – **SiO line decline observed in local SNe**
- **Pure Fe dust does not form efficiently** even in the absence of suphur. In the presence of sulphur, Fe depletion **in FeS for CCSNe**.
- Carbon trapped in CO in PISNe but can be **depleted in AC dust for CCSNe** if He+ is absent.
- Chemical depletion efficiencies and mixing provide a natural limitation to dust formation.

Conclusions

- **Molecules** are abundant in primordial **massive** supernova ejecta with **~ 35 M_{sun}** released to the local gas,
- Our primordial SNe form **less** dust (**1/5**) than in existing models because of the **`chemical bottleneck'**,
- For PISNe, essentially **silica/silicates and pure Si grains. No carbon.** ⟶ other carbon dust providers at z > 6 ? BELCs in quasar winds. WC colliding winds. AGB stars…,
- **Carbon dust** can only form in primitive CCSNe if the environment is **He^+ free** – realistic?
- Mixing and chemical depletion efficiencies are **natural limiting agents** to dust formation and mass yields,
- But PISNe are definitely **molecule and dust providers** to the early universe,

Open questions: Molecule & dust survival in clumps? Sources of **cooling** for PopIII.2 &Pop II.5 star formation? Extinction properties of first galaxies?