Nucleation of Iron Dust from Type II Supernovae

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Abstract

When a star dies in a supernova, its constituent particles are torn apart and a gaseous cloud of atoms remains. These atoms may eventually condense again into large bodies such as planets and stars. There are three main theories as to how this happens: classical, kinetic, and non-local thermodynamic equilibrium (non-LTE). In the classical theory, no nucleation can occur below a critical density and saturation and does not account for much of the nucleation that must occur in the interstellar medium(ISM). The kinetic and non-LTE theories allow for nucleation to occur below the classical critical levels. Most research into this area so far has been focused on the formation of carbon dust. Carbon has a very specific geometry and behaves rather uniquely from a chemical perspective. I was curious as to how a difference in atomic geometry and chemical behavior would affect the formation of dust particles. To investigate this, I am studying the formation of iron dust in supernova remnants. The assumptions that the iron in the supernova remnants exists solely as individual atoms, that the iron atoms are spherical, and that cloud is composed solely of iron atoms all simplified the initial results. Once reasonable results are obtained with these assumptions, they may be removed in order to get a more realistic picture of the formation of iron dust.

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Chapter 1 – Introduction and Background

1.1 Dust Nucleation and Planet Formation

In order for bodies such as stars and planets to form, much smaller particles, or dust, must first form via the process of nucleation from the gaseous remains of supernovae. If these tiny grains of dust manage to attain a minimum, critical size, they may continue to grow. Should the grain just reach the critical size, it may maintain an equilibrium where the number of atoms accreting onto it is exactly equal to the number evaporating away. Anything larger than the critical size will tend to grow, as the amount of stuff attaching to the grain is greater than the amount breaking away. These grains will then attract one another, more and more so as they grow larger and become more significant, and may become lager bodies such as planetoids or, depending on their chemical composition, stars. Many grains never reach this critical size, however, and they will tend to evaporate away.

1.2 Nucleation Models

1.2.1 Classical Model

The classical nucleation model can be applied to a number of phenomena, such as the formation of water vapor into clouds and the growth of sugar crystals into rock candy and essentially assumes a change of thermodynamic state. According to the classical theory, there must already be present an impurity or preformed crystal around which nucleation may occur and the temperature, density, and saturation of the substance in question must be within ideal ranges.

While the requirements of the classical theory are valid if one is watching water freeze into ice, it makes less sense when confronted with the vaporized remnants of a supernova. This very simplified view of the process of nucleation is the starting point of this project.

1.2.2 Kinetic Model

The kinetic theory of nucleation allows nucleation to occur under subsaturated conditions. Generally, the kinetic model predicts higher nucleation rates as it tends not to overpredict the surface free energy of very small grains as the classical model does (Nowakowski & Ruckenstein, 1991). Experimental results for simple alcohols, as seen in Figure 1 for ethanol, show that both the classical and kinetic models are valid under certain conditions and that some other mechanism is needed to understand why the nucleation behavior of these molecules goes from one paradigm to the other.
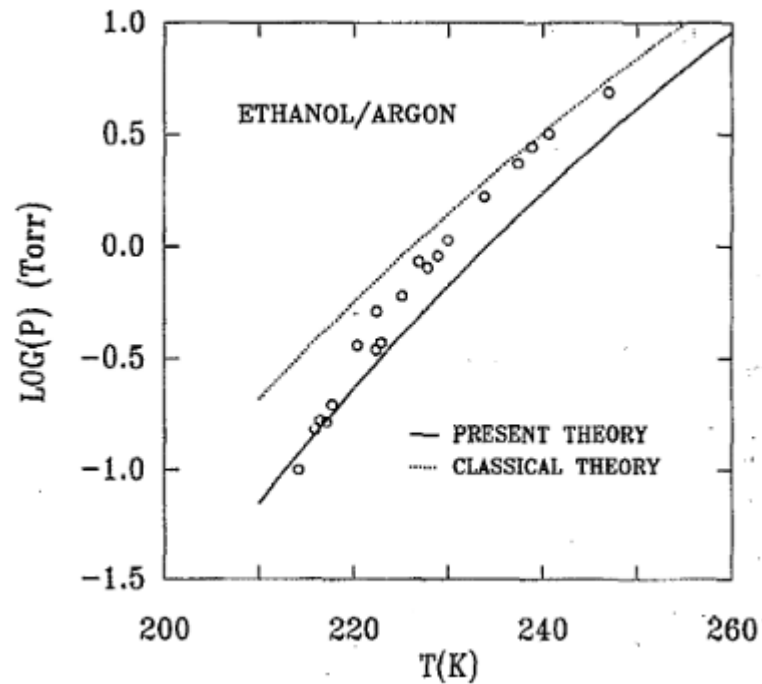
1.2.3 Non-LTE Nucleation

In the classical view, nucleation cannot occur below the critical densities and saturations, both of which depend upon the temperature of the gas cloud in question. However, once saturation and density drop very low, non-local thermodynamic equilibrium nucleation will begin (Lazzati, 2008). In these situations, the temperature of the gas also decreases and the detachment of particles from a grain is suppressed (Lazzati, 2008) allowing nucleation to occur below the classically accepted region.
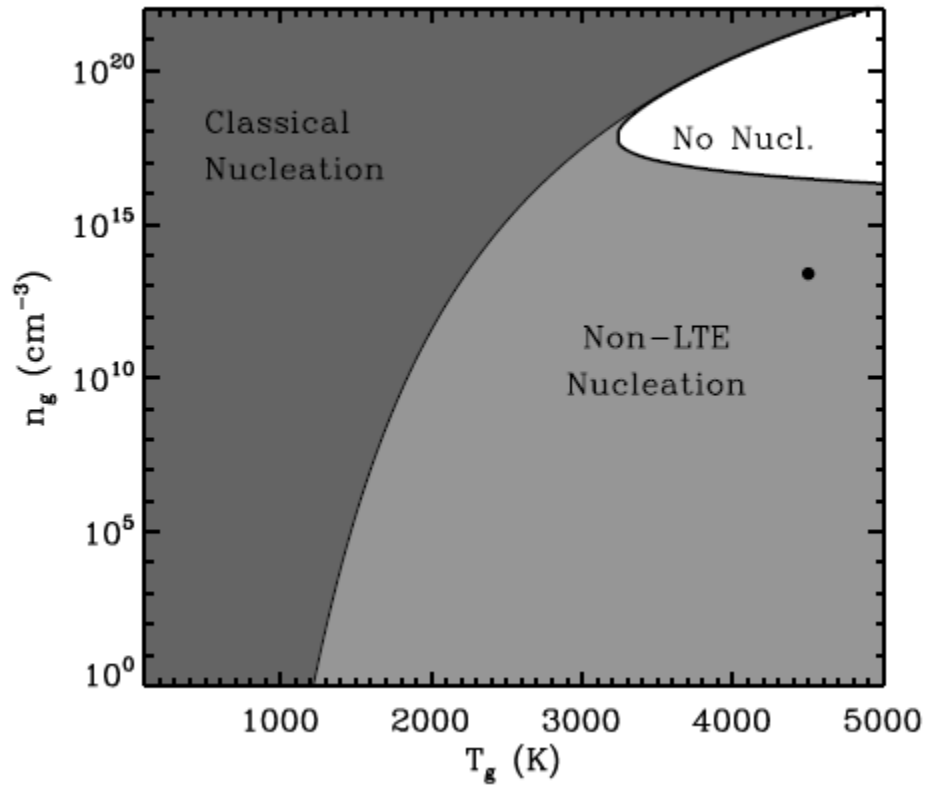
Figure 2 Nucleation diagram for graphite in hydrogen gas (Lazzati, 2008)

Chapter 2 – Methods

2.1 Writing the Program

A computer program was written to simulate the nucleation of iron dust from the interstellar remains of a supernova using Python as the chosen programming language. A majority of the work required to successfully simulate the formation of dust grains came in properly defining variables and constants necessary to calculate the nucleation current

$$J = \alpha\Omega \left(\frac{2\sigma}{\pi m_{lk}} \right)^{\frac{1}{2}} c_{lk}^2 \exp\left[-\frac{4\mu^3}{27\left(\ln S\right)^2} \right]$$

(Todini & Ferrara, 2001). Where m_{lk} is the mass of individual atoms, c_{lk} is the concentration of

atoms in the gas, $\mu = \dfrac{4\pi a_0 \sigma}{k_B T}$, a_0 is the radius of the atoms, σ is the specific surface energy, k_B

is the Boltzmann constant, T is gas temperature, α is the sticking coefficient (which is typically

set to 1), $\Omega = \dfrac{4}{3}\pi a_0^3$ is the volume of a single atom, and S is the supersaturation ration defined

by $\ln S = -\dfrac{\Delta G_r}{RT} + \sum_i v_i \ln P_i$ (Todini & Ferrara, 2001). Ultimately, the nucleation current is

dependent upon the temperature and saturation of the dust cloud, the density of iron particles in

the cloud, and time, meaning that the variables upon which J depends had to be allowed to

depend upon these as well.

A key step in the program had to do with properly varying the density and saturation of the dust

cloud. Over time, the density of particles within the remains of a supernova is reduced by means

of two mechanisms. First, the dust cloud expands over time, increasing the distance between

particles and decreasing the concentration of the cloud. Second, the number of iron atoms left

available to form dust grains decreases as more grains form and as existing grains increase in

size. The saturation of iron particles is a function of the instantaneous density of iron particles in

the cloud and of the critical density required to allow nucleation to occur. This means that only

the equation for density needed to account for both of these mechanisms. Implementing the

dependence of the density on the increasing volume was a simple matter of multiplying the

initial density by the ration of the initial volume to the instantaneous volume. Due to the

complicated dependence of the nucleation rate upon the gas temperature, the reduction of the number of iron particles available to nucleate required the inclusion of both a term describing the number of grains being formed and one describing the addition of new iron atoms to existing grains as a function of the surface area of the grain. This was accomplished using a *for loop* to vary this number as a function of time. The successful implementation of this code produces a very idealized, classical version of the nucleation of iron particles from a gas cloud.

The complete Python code used to generate the results is included as an appendix.

Chapter 3 – Results

3.1 Obstacles and Problems

Once the program was running and all of the pieces were in place, a major road block was finding a range for initial conditions that produced notable results. Initially, the effect of nucleation on the density of the gas cloud was overwhelmed by the change in density due to the expansion of the cloud and was so small as to be negligible. In order to get closer to a realistic model as well as to see meaningful results, the term describing the growth of already formed dust particles was added via

$$dn = c_{lk} \sqrt{\frac{k_B T}{2 \pi m}}$$

(Lazzati, 2008), where dn is the number of particles attaching to the dust grains. This was expected to eat up the iron atoms within the cloud much more quickly than forming new dust particles had. Unfortunately, the output of the program remained essentially unchanged as the

decrease in density and temperature of the cloud were not affected enough by the formation of

dust to produce noticeable results.

3.2 Data and Results

The change in the density, saturation, and temperature of the cloud due only to the change in

volume as a function of the distance from the center of the original supernova explosion can be
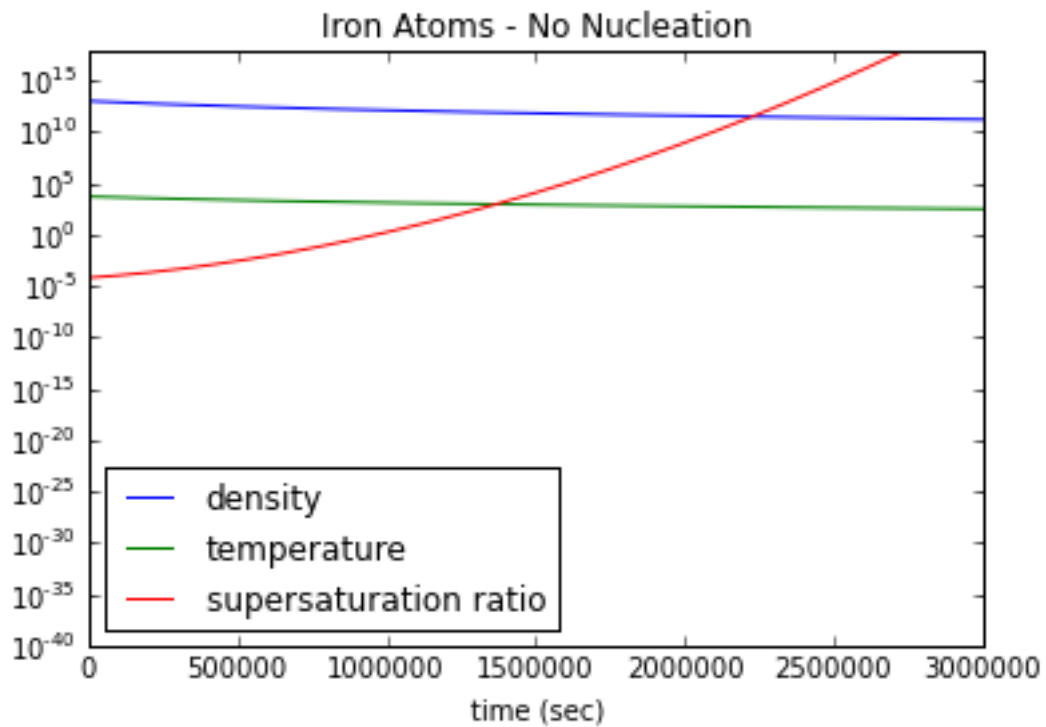
seen modeled in Figure 3.

Figure 3 Evolution of a cloud of iron atoms in which no nucleation takes place

When a term taking into account the nucleation current J was added to the density of the cloud,

the program returned Figure 4 as its output. The supersaturation ratio S is the ratio between the

current density and the critical density for the current temperature; nucleation cannot occur until

S is greater than 1. Once nucleation can happen, it appears to be too small to have a notable
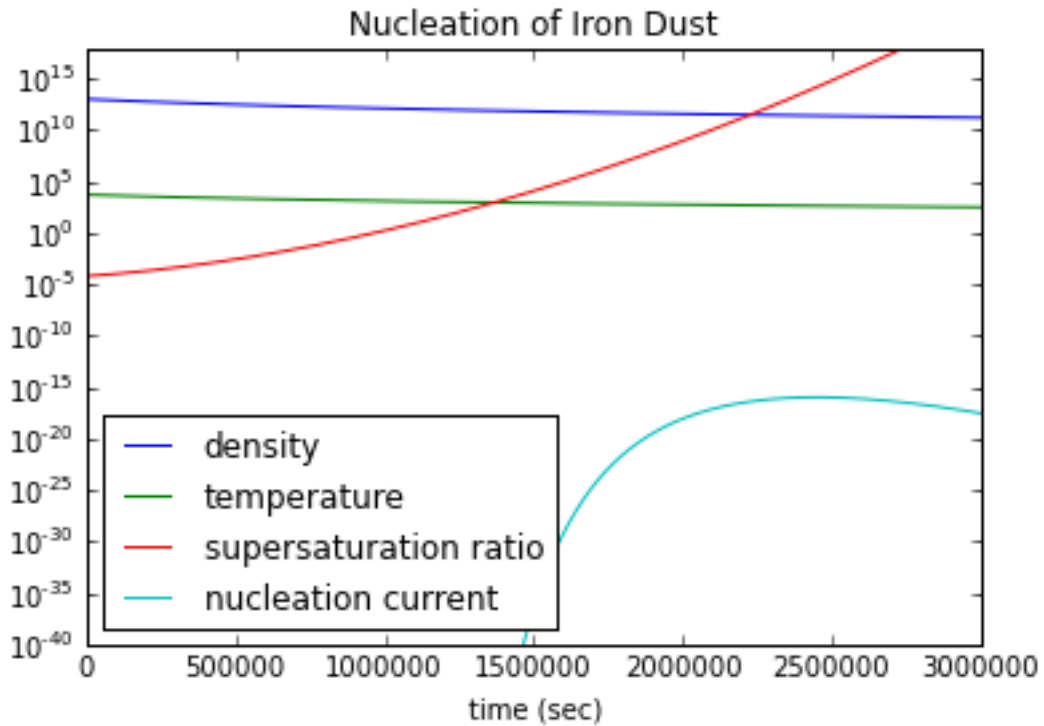
effect on the density curve.

Figure 4 Evolution of a cloud of iron atoms including the formation of dust particles

Chapter 4 – Analysis and Discussion

4.1 Data Analysis

My results do not seem to indicate that the formation of dust particles from a cloud of iron atoms

has any notable effect on the density, saturation, or temperature of the cloud. A number of

changes to the initial conditions and to the syntax and formatting of the equations in the program

all yielded the same results. The beginning stages of nucleation, i.e. the formation of dust grains

of more than one atom of iron, will have little to no effect on the cloud. One would assume that

the growth of these grains up to and beyond the critical radius will have a much more dramatic effect on the could as a whole, as larger and larger grains will have more surface areas for the free atoms and smaller grains to stick to.

Chapter 5 – Conclusion

5.1 Conclusions

The very simplified model of nucleation that my program demonstrates does not take into account the vast majority of what must be really happening as stars and planets form from the remnants of supernovas. The beginning stages of the formation of dust grains does not have enough of an effect on the density of the cloud to be observed. Moving forward, the inclusion of equations representing more aspects of the phenomenon should begin to yield notable results.

5.2 Future Research

Ideally, an accurate to observation model of iron dust nucleation will be realized by continuing to add complications into a system like the one I have begun. These would include the effects of not only classical nucleation, but also the kinetic and non-LTE effects at lower temperatures, densities, and saturations of the ISM as well as other effects we have yet to observe or model. The immediate next step would be to include in the program a term representing the growth of the dust grains up to and beyond the critical size and another demonstrating the detachment of particles from the growing grains. As in most areas of physics, one may approach a model very similar to the actual process by which gases and dust become planets and stars, but the true model will include many more effects than we can realistically account for.

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List of Figures

Appendix

Following is the text of the program used to generate the results presented herein.

```
import numpy as n

import pylab as p

from math import pi

from math import exp

from math import log

def crit_dens(T):

        kB=1.38e-16 # Boltzmann's constant in CGS

        logPPa=12.106-21723./T+0.4536*n.log(T)-0.5846*T**(-3)*.01        # from Wikipedia

        Pres=n.exp(logPPa)

        dens=Pres/kB/T

        return dens

volume0=1.                      # the volume of the nucleating region at t=0

density0=1e13                   # the numeric density (atoms per cm3) of iron at t=0

temperature0=5000.              # the temperature in Kelvin at t=0

velocity=100.*1e5               # the expansion velocity of the gas parcel in cm/s

distance0=1e13                  # initial distance in cm from the center of the SN explosion
```

```
# Some constant values for Iron

sigma=1800.                     # the surface tension of Iron in erg/cm^2

a0=1.411e-8                     # interatomic radius in cm

omega=4./3.*n.pi*a0**3         #vol of a molecule in condensed phase in cm^3

alpha=1.                       #sticking coefficient

m=9.27e-23                     #mass of iron atom in g

kB=1.38e-16                    #Boltzmann's constant


# set time base for numerical integration

dt=100.                        # the time interval in seconds

tmin=0.                        # the initial time in seconds

tmax=3000000.                  # the final time in seconds

times=n.arange(tmin,tmax+dt/2.,dt)  # the array of times

nt=times.size                  # the number of elements in the time array


# calculating quantities as a function of time

distance=distance0+velocity*times

volume=volume0*(distance/distance0)**3

temperature=temperature0*(volume0/volume)**(2./3.)


# calculating the critical density at various temperatures

crit_density=n.empty(nt)
for i in range(nt):
        crit_density[i]=crit_dens(temperature[i])

density=n.zeros(nt)
```

```python
    r_critical=n.zeros(nt)
    saturation=n.zeros(nt)
    J=n.zeros(nt)
    drhoNucl=n.zeros(nt)
    density[0]=density0
    for i in range(1,nt):

    dV=volume[i]-volume[i-1]
            d_density=-density[i-1]/volume[i-1]*dV
            saturation[i]=density[i-1]/crit_density[i-1]
            r_critical[i]=2.*sigma*omega/(kB*temperature[i]*n.log(saturation[i]))
            # dA=4.*n.pi*(r_critical[i])**2.-4.*n.pi*(r_critical[i-1])**2
            # dn=density[i-1]*(kB*temperature[i]/(2*n.pi*m))**.5*dt*dA        #Terms to be used
                                                                              later when adding the
                                                                              effect of grain growth


            mu=4*n.pi*a0**2*sigma/kB/temperature[i]
            if saturation[i]>1: J[i]=alpha*omega*(2.*sigma/(n.pi*m))**.5*density[i-1]**2*n.exp(-
            4*mu**3/(27.*n.log(saturation[i])**2))
            else: J[i]=0
            drhoNucl[i]=4./3.*n.pi*(r_critical[i])**3/omega*J[i]*dt
            density[i]=density[i-1]+d_density-drhoNucl[i]

    jj=n.where(saturation<1)
    J[jj]=0

    # plotting results

    p.close(1)
    p.figure(1)
    p.title('Iron Nucleation')
    p.semilogy(times,density,label='density')
    p.plot(times,temperature,label='temperature')
    p.plot(times,saturation,label='supersaturation ratio')
    p.plot(times,J,label='nucleation current')
    p.xlabel('time (sec)')
    p.legend(loc='lower left')
    p.ylim([1e-40,1e18])
    p.show()
```