Spiral Molecular Front in Galaxies: Quick
Transition from Atomic to Molecular Hydrogen in
Spiral Arms

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Abstract

We derived a two-dimensional map of the molecular fraction, $f_{\text{mol}}$, (ratio of the molecular gas density to that of total gas) in the spiral galaxy M51, and examined the behavior of molecular fronts (MF), where MF represents the place where $f_{\text{mol}}$ changes drastically from nearly zero to unity and vice versa. We show that the MF phenomenon occurs not only radial, but also in the azimuth direction through the spiral arms, and $f_{\text{mol}}$ changes rapidly in the arm-to-inter-arm transition regions. The existence of the azimuthal MF indicates that the atomic gas (HI) is quickly transformed to molecular gas ($H_2$) during the passage through spiral arms. We performed a numerical simulation of MF based on an HI-to-$H_2$ phase transition theory, and reproduced the observations. We estimated a azimuthal scale length of the transition to be less than 200 pc, corresponding to a time scale of $\sim 2$ Myr for $H_2$ gas formation. The azimuthal width of a molecular arm is estimated to be at most 2.5 kpc, where the gas can remain in molecular phase for about 25 Myr.

Kew words: galaxies: spiral — galaxies: ISM — galaxies: cluster of — Molecular gas — HI gas

1 Introduction

The neutral (HI) and molecular hydrogen ($H_2$) gases are the two major components of the interstellar matter. Elmegreen (1993) has proposed a simple model to predict the molecular fraction by assuming a quasi-static equilibrium between the two phases in individual interstellar clouds. However, the dynamical transition between HI and $H_2$ gas phases are not well understood in real galaxies: Are the GMCs (giant molecular clouds) long-lived clouds living for several galactic rotations crossing the
spiral arms for many times, coexisting with the HI gas? Alternatively, are they formed quickly from HI gas when the inter-arm HI encounters the arms, and does molecular gas return to HI again, when going out of the arms?

This question can be answered by studying the distribution of molecular fraction, the ratio of molecular-gas density to the total gas density, in the gas disk of spiral galaxies. Global variations of the molecular fraction in disk galaxies have been obtained by our earlier works (Sofue et al 1995; Honma et al 1995), applying the Elmegreen’s theory of atomic-to-molecular gas transition. We showed that the inner gas disk is dominated by molecular gas, while the outer disk by HI, and the transition between HI and H$_2$ occurs in a narrow annulus in the disk, across which the molecular fraction varies drastically. We call this transition region the “molecular front (MF)”. Such front phenomenon was found also in the direction perpendicular to the galactic plane, so that the H$_2$ disk is sandwiched by a fat HI disk (Imamura and Sofue 1997). However, these analyses do not tell us about dynamics and time scale of the HI-to-H$_2$ transition.

In the present paper, we investigate the MF phenomenon across spiral arms by obtaining a two-dimensional distribution of molecular fraction in a galactic disk. Azimuthal variation of molecular fraction across spiral arms will provide us with information about dynamical evolution of the HI-H$_2$ phase transition and molecular gas formation in spiral arms.

2 Molecular Front

2.0.1 Radial and Vertical Molecular Front

Many observations of the neutral hydrogen and the molecular gas have been carried out, and have revealed two important aspects. First, the neutral hydrogen gas is broadly distributed in the disk, and is often extended outside the optical disks, while it is deficient in the central regions. On the other hand, molecular gases are concentrated in the central a few kpc regions. The radial variation of the distributions of HI and H$_2$ gases have been quantified by analyzing the molecular fraction as a function of the galactocentric distance. The molecular fraction, $f_{\text{mol}}$, is defined by

$$f_{\text{mol}} = \frac{\rho(H_2)}{\rho(\text{HI}) + \rho(H_2)} = \frac{2 \times n(H_2)}{n(\text{HI}) + 2 \times n(H_2)}. \quad (1)$$

Sofue et al. (1995) have investigated radial variation of the molecular fraction in several spiral galaxies. They found that the molecular fraction is almost unity in the central a few kpc region, and decreases suddenly at a certain radius to almost zero, beyond which the gas is almost totally in the HI phase. Such a step-like variation of the molecular fraction is called the molecular front.

Honma et al. (1995) modeled the molecular front by applying the phase transition theory of Elmegreen (1993). According to this theory, the molecular fraction is determined by three parameters: interstellar pressure $P$, UV radiation field $U$, and
metallicity $Z$. Honma et al showed that, if these three parameters are approximated by exponential functions of galacto-centric radius, the observed molecular front in the radial direction can be well reproduced. They applied this model to several real galaxies, and obtained good coincidence with observed data.

Spiral galaxies have density waves and spiral arms. As the spiral pattern speed is much slower than the gas’s rotation, the gases collide with the spiral potential, resulting in galactic shock waves, where the gas density and pressure increase suddenly. The compression results in star formation, leading to increase of the radiation field intensity. Thus, the MF parameters, $(P, U, Z)$, will vary as a function of azimuthal angle, which may results in another type MF spatially correlated with the spiral arms. In order to investigate the existence of such spiral MF, we first examine the HI and CO-line data from the literature, and construct a 2D map of the molecular fraction in M51. Then, we perform numerical simulation using the transition model established by Elmegreen (1993), and compare with the observations.

### 2.1 Spiral Molecular Front in M51: Azimuthal Variation of Molecular Fraction

For obtaining two-dimensional map of molecular fraction, we make use of the data from the literature that provide sufficient angular resolution in both HI and CO. Here, we choose the ‘grand-design’ spiral galaxy NGC 5194 (M51), which was also studied in Honma et al. (1995). We use the $^{12}$CO $(J = 1 - 0)$ imaging data obtained with the Nobeyama 45-m telescope (Nakai et al 1994) with the beam width of 16″ and grid spacing of 15″, corresponding to an angular resolution of 24″, and the HI data obtained with the VLA at 34″ × 34″ resolution from Rots et al. (1990). Integrated-intensity maps of HI and CO are shown in Fig. 1 at the same resolution of 34″. These two maps reveal the typical behaviors of atomic and molecular hydrogen gases: HI is extended broadly in the disk, having central deficient, while CO is concentrated in the central region.

![Fig. 1](image)

We calculate the column density of HI and $H_2$ from the integrated intensity, adopting the following relation between the column density and intensity:

\[
\begin{align*}
n(\text{HI}) &= C(\text{HI}) \times I(\text{HI}), \\
n(\text{H}_2) &= C(\text{CO}) \times I(\text{CO}),
\end{align*}
\]

where $C(\text{HI})$ and $C(\text{CO})$ are the conversion factors. The value of $C(\text{HI})$ can be easily calculated as $1.82 \times 10^{18}$ cm$^{-2}$ K$^{-1}$ km$^{-1}$ sec. In order to estimate the amount of the total molecular gas mass from CO intensity, we adopt a conversion factor of $C(\text{CO}) = 1.1 \times 10^{20}$ cm$^{-2}$ K$^{-1}$ km$^{-1}$ sec from Arimoto et al. (1996), and assume no radial dependence of the conversion factor. The difference of the angular resolution was corrected, so that both HI and CO maps have the same resolution of 34″, and the grid separation was corrected by using bicubic interpolation. Using Eq. 1, we
calculated the molecular fraction, and show a two dimensional distribution map of the molecular fraction in Fig. 2.

Fig. 2 shows that the molecular fraction is almost unity in the central \( r < 60'' \) region, or at \( r < 2.8 \) kpc. Toward the northwest and southeast, where the bisymmetric spiral structure is not seen clearly in both HI and CO distribution, the molecular fraction decreases drastically to zero at \( r > 110'' \), or \( r > 5.1 \) kpc. This sudden radial decrease of the molecular fraction confirms the radial MF at \( r \sim 5 \) kpc.

In the northeast and southwest, where the molecular spiral arms are prominent, a high-\( f_{\text{mol}} \) region extends until \( \sim 7 \) kpc. In the southeast direction, \( f_{\text{mol}} \) suddenly decreases to 0.6 at \( r \sim 60'' \), and increases again to a value greater than 0.9, and finally decreases to zero. This re-increase of the molecular fraction results from the spiral arms, as already mentioned by Kuno et al. (1997).

Fig. 2 shows that the molecular front exists along the spiral arms in addition to the global radial variation. This implies that the circularly flowing gas experiences quick transition from atom to molecule by encountering the spiral arms, and from molecule to atom when going out from the spiral arms. However, the present angular resolution is not high enough to investigate the scale length of the variation across the arms in more detail. We can estimate only the upper limit of the scale length, which is about 700 pc in the azimuthal direction. Since the rotation velocity is about 200 km/sec (Kuno & Nakai 1997) and pattern speed of the density waves will be \( \sim 20 \) km s\(^{-1}\) kpc\(^{-1}\), the upper limit of time scale of atom-to-molecule and molecule-to-atom phase transitions is estimated to be several Myr.

### 3 Simulation of the Molecular Front

#### 3.1 Numerical Methods

In previous section, we have shown the existence of MF in azimuthal direction. However, because of poor angular resolution, we could not estimate the exact MF scale length in the arms. Here, we try to estimate the scale length by numerical simulations. The azimuthal variances of the gas density is calculated using the hydrodynamical code, not taking into account the self-gravity of the gas. The variation of metallicity and radiation field is assumed to have an axisymmetric exponential distribution, as adopted by Honma et al. (1995), but no azimuthal variation is assumed.

For calculating the gas dynamical behavior of the disk, we use the freely downloadable and usable hydrodynamical code, VH-1 (Blondin & Lufkin 1993). This is a multidimensional hydrodynamics code for an ideal compressible fluid written in FORTRAN, developed by the numerical astrophysics group at the University of Virginia on the bases of the Piecewise Parabolic Method Lagrangian Remap (PPMLR)
scheme of Colella & Woodward (1984). The PPMLR has the advantage of maintaining contact discontinuities without the aid of a contact steepener, and is good to be applied to a galactic scale hydrodynamical simulation. The code does not include self-gravity, artificial viscosity, variable gamma equation of state, and radiative heating and/or cooling. Hence, we assume that the interstellar gas is ideal, inviscid, and compressible.

3.1.1 Gravitational Potential

In order to simulate the evolution of spiral structure in the gas disk, we assume a given gravitational potential, which comprises the following two terms: (i) a static axisymmetric potential, and (ii) a nonaxisymmetric, rotating bar potential. The self-gravity of the gas is not taken into account. The potential is expressed by

$$\Phi(R, \phi) = \Phi_0(R) + \Phi_1(R, \phi).$$

(4)

We adopt a “Toomre disk” (Toomre 1981) potential for the axisymmetric component as given by:

$$\Phi_0(R) = -\frac{c^2}{a} \frac{1}{(R^2 + a^2)^{1/2}},$$

(5)

where $a$ is the core radius, and $c = \frac{v_{max}(27/4)^{1/4}}{a}$ with $v_{max}$ being the maximum rotation velocity. Through our numerical simulation, we fix the core radius and maximum circular velocity to be $a = \sqrt{2}$ kpc and $v_{max} = 200$ km s$^{-1}$.

The nonaxisymmetric potential is taken from Sanders (1977), assuming rigid rotation at a pattern speed $\Omega_p$, which has the form

$$\Phi_1(R, \phi) = \varepsilon \frac{aR^2}{(R^2 + a^2)^{3/2}} \Phi_0(R) \cos 2 (\phi - \Omega_p t),$$

(6)

where $\varepsilon$ is the strength of the bar of the order of $\varepsilon = 0.15$. Spiral shocked arms of gas are produced by this potential.

3.1.2 Initial Condition

Initially, we set $256 \times 256$ two-dimensional cells corresponding to $12.8 \times 12.8$ kpc field, setting the field center at the coordinates origin. The initial number density of the gas is taken to be $5$ cm$^{-1}$ for the inner disk at $R \leq 8$ kpc, and $1$ cm$^{-1}$ at $R > 8$ kpc. Initial rotation velocity of each gas cell is set so as for the centrifugal force to balance the gravitation. The bar pattern speed $\Omega_p$ is taken to be $23$ km s$^{-1}$ kpc$^{-1}$, and the strength of the bar $\varepsilon$ is taken to be $0.10$.

3.2 Elmegreen’s Parameters

We specify three parameters: interstellar pressure $P$, radiation field strength $U$, and metallicity $Z$. Following Honma et al. (1995), we represent $U$ and $Z$ by the
following equations.

\[
\frac{U}{U_\odot} = \exp \left( -\frac{R - R_{U_*}}{R_U} \right),
\]

\[
\frac{Z}{Z_\odot} = \exp \left( -\frac{R - R_{Z_*}}{R_Z} \right).
\]

Here, \( R_U \) and \( R_Z \) are the scale radii of the radiation field and metallicity, respectively, and \( R_{U_*} \) and \( R_{Z_*} \) are the radii at which the quantities are normalized to the solar values.

It is possible that radiation field depends on the azimuthal direction, because star formation along the spiral arms is enhanced and newly born OB stars radiate strong UV emission. Thus, it seems that there is little UV radiation in the inter-arm regions. However, Greenawalt et al. (1998) presented deep H\( \alpha \) emission-line images of several spiral galaxies including M51, concluding that a half of total H\( \alpha \) emission is contributed by the diffuse ionized gas. This observation shows that the fluctuation of ionizing radiation field in arm and inter-arm regions is not more than twice at their resolution of a few arcsecs. In the present simulation, the resolution is much lower, and the arm-interarm UV fields may be assumed to have intensity fluctuation less than twice: We here assume that the UV field is uniform along an azimuthal circle, and depends only on the galactocentric distance. Although they are a scope beyond the present paper and will be subject for simulations in the future, variation of radiation fields by star-forming arms should be taken into account, and UV radiation transfer through the arms, particularly through dark lanes, should be solved, in order to obtain a more realistic, higher resolution behavior of the molecular-fraction across spiral arms.

The interstellar pressure is estimated as \( P \propto \rho \text{(gas)} \), in the same manner as Honma et al. (1995), and express it by the following relation:

\[
\frac{P}{P_\odot} \sim \frac{\rho}{\rho_\odot}.
\]

We adopt the following normalizing parameters: \( \rho_\odot = 2H\text{cm}^{-3} \), \( R_U = R_Z = 5.2 \) kpc, and \( R_{U_*} = R_{Z_*} = 11.5 \) kpc. The latter two parameters are as same as those assumed by Honma et al. (1995). Although they assumed constant metallicity for NGC 5194, we here assume an exponential function as above (see e.g. Arimoto et al 1996).

\subsection*{3.3 Simulated Spiral Molecular Front}

Under these assumptions and initial conditions, we first calculated the time evolution of the distribution of total gas. Fig. 3a shows the density distribution after several galactic rotations. The density distribution in the initially uniform-density disk is strongly disturbed by the oval potential, and high-density arms are formed, which
evolve into well-developed bisymmetric spiral arms. In the same time, the global radial density distribution is regulated to have a roughly exponentially-decreasing structure. Inside the bar, straight high-density arms are formed along the axis of the bar, as well as many faint spiral-like arms. We are here interested in the global spiral pattern in order to compare with the observed gas density distributions, and will not discuss the smaller and fainter features, which will be finally smeared out when we compare the result with the observation.

— Fig. 3a, b, c, d —

The simulated distribution of gas density is, then, used to calculated the distribution of gas pressure $P$, which is further combined with the assumed distributions of UV radiation field $U$ and the metallicity $Z$ as given above. Thus, we can calculated the molecular fraction at each grid point, and obtain a map of $f_{\text{mol}}$, as well as maps of atomic and molecular gases. Fig. 3b, c and d shows snapshots of the thus calculated maps for HI, $H_2$ and $f_{\text{mol}}$. In order to compare with the observations, we smooth the map of molecular fraction by a Gaussian convolution, and compare it with the observation of M51 in the same resolution in Fig. 4.

— Fig. 4 —

4 Discussion

The simulated results can be summarized as follows. Detailed arm shapes are not well reproduced, because the simulation uses a fixed bar-potential. In order for detailed arm features to be reproduced, we need self-gravitating $N$-body simulation, including both stars and gas, is necessary, which is a subject for the future. However, the simulation in Fig. 3 and 4 shows global agreement with the observations, and reproduces the following characteristics of the distribution of molecular fraction in M51. Around the nucleus $f_{\text{mol}}$ is almost unity, and maintains high values $r \sim 4$ kpc, where $f_{\text{mol}} > 0.8$. At $r \sim 4$ to 5 kpc, $f_{\text{mol}}$ decreases drastically to 0.4 or lower, and becomes nearly zero in the outer region. It is clear that the transition region, where $f_{\text{mol}}$ is $\sim 0.5 - 0.6$, is distributed in a narrow annulus of radius of 4.5 kpc, which means that the HI-to-$H_2$ transition occurs rather abruptly within a narrow range of radius. This confirms the radial molecular front (Sofue et al. 1995, Honma et al. 1995).

In addition to the radial MF in the gas disk, azimuthal fluctuation of molecular fraction is also significant. At $r \sim 6$ kpc, $f_{\text{mol}}$ changes from nearly zero before encountering the arm to $\sim 0.8$ within $\sim 200$ pc in the azimuthal direction in the spiral arm. This narrow transition range corresponds to a time scale of $\sim 2$ Myr. This indicates that the molecular gas observed along spiral arms is formed only within $\sim 2$ Myr. This time scale is consistent with the $H_2$ forming time scale $> 7 \times 10^5$ yr predicted by Takahashi & Williams (2000) using a molecular dynamics simulation.

On the other hand, the decaying time scale of molecular gas is longer, according
to the more gradual decrease of gas density after the galactic shock passage. If we define a molecular arm an armed region with $f_{\text{mol}} > 0.5$, the width of the molecular arm is estimated to be $\sim 2.5$ kpc in the azimuthal direction. This corresponds to a lifetime of molecular gas of about 25 Myr, which is consistent with the semi-analytically calculated GMCs lifetimes $\sim 40$ Myr (Elmegreen 1991).

If we consider the radial variation of metallicity $Z$, these local (arm) $f_{\text{mol}}$ structures will depend on the galactocentric distance, even for the same gas density. Fig. 3 shows that, for the same density of $\sim 5$ H cm$^{-3}$, the molecular fraction is $\sim 0.5 – 0.6$ in the inner inter-arm region, while it is $0.3 – 0.4$ in the outer arm regions. This reflects the fact that the molecular fraction depends not only on the gas density, but also on the strength of radiation field and metallicity, particularly the latter.

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Figure Captions

Fig. 1. (a) HI integrated-intensity map of NGC 5194 (M51) at 34″ resolution (Rots et al. 1990) (left panel). The contour levels are 100, 300, 500, . . . , and 1900 mJy/beam and the intensity key is shown at the bottom.
(b) $^{12}$CO ($J = 1 - 0$) integrated intensity map of M51 (Nakai et al. 1994), smoothed to the same spatial resolution (34″) as that of HI. The contour interval is 6.6 K km sec$^{-1}$, and the intensity key is shown at the bottom. 10″ in the maps correspond to linear scale of 466 pc.

Fig. 2. Molecular fraction ($f_{mol}$) in NGC 5194 (M51). Contour levels are $f_{mol} = 0.1, 0.2, . . . , 0.9$.

Fig. 3. (a) A snapshot of numerically simulated total density distribution of interstellar gas.
(b) The same for HI gas.
(c) The same for H$_2$ molecular gas, simulating a CO-line intensity distribution.
(d) The same for molecular fraction $f_{mol}$.
The value keys are shown at the bottom.

Fig. 4. Comparison of the simulated molecular fraction (left) smoothed to the same resolution as that of the observation of M51 (right).
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