

THEORETICAL CONSIDERATIONS OF SHOCK WAVE BEHAVIOR

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Interstellar shock waves have a significant influence on the structure and dynamics of interstellar matter and probably trigger star formation in suitably dense regions. In this paper the overall structure of regions near shock waves is reviewed. In addition we discuss the main observational effects of shocks on interstellar molecules, including: (i) acceleration to velocities $1 \text{ km s}^{-1} < v_s < 100 \text{ km s}^{-1}$ relative to the ambient gas, (ii) excitation of infrared lines in the heated postshock gas, and (iii) production of high abundances of certain molecular species such as H, OH, H₂O, CH⁺, OCS, and SiO through high temperature chemical reactions in the $T \gtrsim 1000 \text{ K}$ postshock gas. The molecular region around the BN infrared source in Orion and the high velocity molecules in IC443 are discussed as possible examples of shocked molecular gas.

1. INTRODUCTION

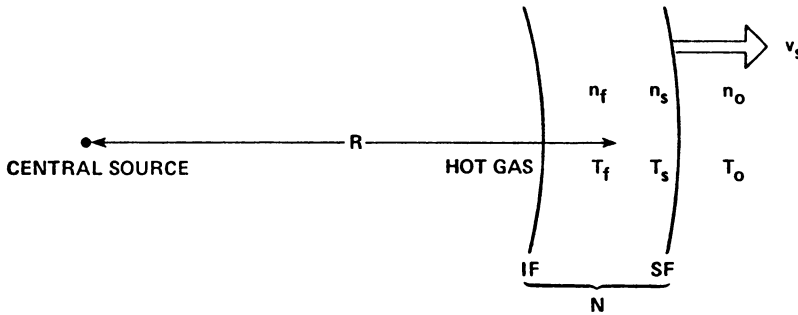
Shock waves in the interstellar medium may induce star formation (e.g., Shu, Milione and Roberts 1973, Elmegreen and Lada 1977, Herbst and Assousa 1977, and Loren and Vrba 1979) and may play a significant role in determining the density, temperature and velocity structure of the interstellar medium (e.g., Heiles 1979, McKee and Ostriker 1977, Norman and Silk 1979). Besides their presence in spiral density waves and cloud-cloud collisions, interstellar shocks frequently accompany the birth and death of stars, and they may persist throughout the life of massive stars: stellar winds, expanding HII regions, and supernova remnants are all capable of driving shock waves.

The purpose of this paper is to review the overall structure near interstellar shock waves and to focus on the interaction of shocks with interstellar molecules. Shock waves change the relative chemical abundances of molecules (primarily through enhancements in both dissociation and formation rates at the elevated postshock temperatures), collisionally excite rotational and vibrational transitions of the molecules in the warm postshock gas, and accelerate molecules to

supersonic velocities. The high excitation and the velocity shift of the postshock molecules not only serve as shock signatures but reduce the absorption in the lines caused by any surrounding cold molecular gas, making detection much simpler.

2. LARGE-SCALE STRUCTURE OF SHOCKED SHELLS

The time dependent large-scale structure of the interstellar medium interacting with supernova remnants, stellar winds, or HII regions can be analytically formulated if the approximation of an initial constant hydrogen nucleus density n_0 is assumed. A shock front (SF) is established behind which, once it has slowed to $v_s < v_c$, the shocked ambient gas radiatively cools and forms a neutral shell, bounded on the inside by an ionization front (IF). (See Figure 1.) The hydrogen nucleus column density N in the shell, the radius of the shell R , and the timescale t are functions of the velocity of the shell; solutions have been obtained for HII regions (Spitzer 1968), supernova remnants (Woltjer 1973) and early-type stellar winds (Castor, McCray and Weaver 1975) and are summarized in Figure 1 along with the critical



	HII REGIONS	WINDS	SN
v_{cr} (km s ⁻¹)	14	$76 n_3^{1/5} L_W^{3/5} L_{48}^{-2/5}$	$516 n_3^{2/17} E_{51}^{1/17}$
t (yr)	$3.1 \times 10^4 v_{s6}^{-7/3} n_3^{-2/3} L_{48}^{1/3}$	$9.7 \times 10^4 v_{s6}^{-5/2} n_3^{-1/2} L_W^{1/2}$	$1.1 \times 10^5 v_{s6}^{-4/3} n_3^{-19/51} E_{51}^{16/51}$
R (pc)	$0.36 v_{s6}^{-4/3} n_3^{-2/3} L_{48}^{1/3}$	$1.6 v_{s6}^{-3/2} n_3^{-1/2} L_W^{1/2}$	$4.5 v_{s6}^{-1/3} n_3^{-19/51} E_{51}^{16/51}$
N (cm ⁻²)	$3.6 \times 10^{20} v_{s6}^{-4/3} n_3^{1/3} L_{48}^{1/3}$	$1.6 \times 10^{21} v_{s6}^{-3/2} n_3^{1/2} L_W^{1/2}$	$4.5 \times 10^{21} v_{s6}^{-1/3} n_3^{32/51} E_{51}^{16/51}$

$n_3 = n_0 / 10^3 \text{ cm}^{-3}$

$v_{s6} = v_s / 10 \text{ km s}^{-1}$

$E_{51} = \text{INJECTION ENERGY IN } 10^{51} \text{ erg}$

$L_{48} = L_i / 10^{48} \text{ s}^{-1}$

$L_W = \text{WIND LUMINOSITY IN } 10^{36} \text{ erg s}^{-1}$

Figure 1. Large-scale structure near shock waves

velocity v_c . We note that Hill and Hollenbach (1978) have shown that around typical expanding HII regions, the FUV photon flux from the central stars dissociates molecules ahead of the shock front until it has slowed to $v_s \lesssim 3 \text{ km s}^{-1}$.

3. THE EFFECT OF SHOCK WAVES ON INTERSTELLAR MOLECULES

3.1 Dissociative and non-dissociative shocks

Shocks can be divided into two regimes for the purposes of studying the effect of shocks on molecules: (i) non-dissociative shocks ($v_s \ll 30 \text{ km s}^{-1}$) which mainly heat the ambient molecules and create new molecular abundance ratios by the effects of increased postshock density and temperature on the formation rates of key molecules, and (ii) dissociative shocks ($v_s \gg 30 \text{ km s}^{-1}$) which fully dissociate any pre-existing molecules, but which reform molecules in the cooling $T < 5000 \text{ K}$ postshock gas. The exact velocity v_d at which molecules are dissociated has been thrown into question recently by Dalgarno and Roberge (1979), who show the dissociation rate coefficients for molecules to be quite density sensitive. Until more quantitative calculations are performed, v_d can be bracketed by its high density ($n_0 \gtrsim 10^{10} \text{ cm}^{-3}$) value of approximately 25 km s^{-1} (Kwan 1977) and a low density ($n_0 \rightarrow 0 \text{ cm}^{-3}$) value of probably less than 50 km s^{-1} , since the postshock collisional ionization will produce a sufficient fractional abundance of electrons, $x(e) \sim 0.2$ (Shutt and McKee 1979), to collisionally dissociate H_2 .

3.2 Overview of postshock structure

Dissociative and non-dissociative shocks have certain overall similarities. Shocked gas is initially heated and later cooled and compressed as it moves downstream from the shock front. The immediate postshock kinetic temperature T_s is

$$T_s = 3.2 \times 10^5 x_{ts}^{-1} v_{s7}^2 \text{ K}, \quad (1)$$

where $v_{s7} = v_s/100 \text{ km s}^{-1}$ and x_{ts} is the number of gas particles per proton; $x_{ts} = 2.3$ for ionizing shocks with $v_{s7} \gtrsim 1$, $x_{ts} = 0.6$ for non-dissociative shocks into molecular ambient gas. Downstream the gas cools and compresses ($nT \sim \text{constant}$) until magnetic pressure dominates and compression ceases at density n_f .

$$n_f = 77 v_{s7} B_{\mu G}^{-1} n_0^{1/2} \text{ cm}^{-3}, \quad (2)$$

where $B_{\mu G}$ is the ambient magnetic field in μGauss and n_0 is in cm^{-3} . Cooling continues to equilibrium $T_f \sim 10 - 100 \text{ K}$.

However, despite these overall similarities, the detailed postshock structure behind dissociative shocks is quite different from non-dissociative shocks. The high postshock temperatures ($T \sim 10^5 \text{ K}$)

behind fast shocks leads to high levels of ionization and UV cooling to $T \sim 10^4$ K in a column density $N_{\text{cool}} \sim 2.1 \times 10^{17} v_{s7}^{4.2} \text{ cm}^{-2}$ (Shull and McKee 1979, Hollenbach and McKee 1979a). Initial calculations by Hollenbach and McKee (1979b) suggest that for $n_0 \lesssim 10^3 \text{ cm}^{-3}$ the gas cools from 10^4 K to 100 K primarily by the CII(156 μ) and OI(63 μ) lines in a column density $N_h \sim 10^{19} \text{ cm}^{-2}$; the column density of warm ($T > 100$ K) H_2 is of order $N_2 \sim 10^{16} \text{ cm}^{-2}$. Column densities of warm CO, H_2O , and OH are less than 10^{12} cm^{-2} . Complete reformation of the molecules occurs in a column density $N_m \sim 10^{21} \text{ cm}^{-2}$ in the cool ($T < 100$ K) gas. UV absorption or radio measurements would generally detect this cold postshock gas; infrared emission measurements could not detect the warm postshock gas at present sensitivity. On the other hand, when $n_0 \gtrsim 10^4 \text{ cm}^{-3}$, the gas behind fast shocks cools to 100 K in a column density $N_h \sim 10^{21}$ to 10^{23} cm^{-2} , the greater column density being in part due to reduced cooling rates caused by collisional suppression of atomic and molecular lines and in part due to significant heating by H_2 formation. Molecular hydrogen formation on grains is less efficient at higher gas and grain temperatures so that the column density for complete molecular reformation is also $N_m \sim 10^{21}$ to 10^{23} cm^{-2} . The postshock structure of fast, dissociative shocks is summarized in Figure 2.

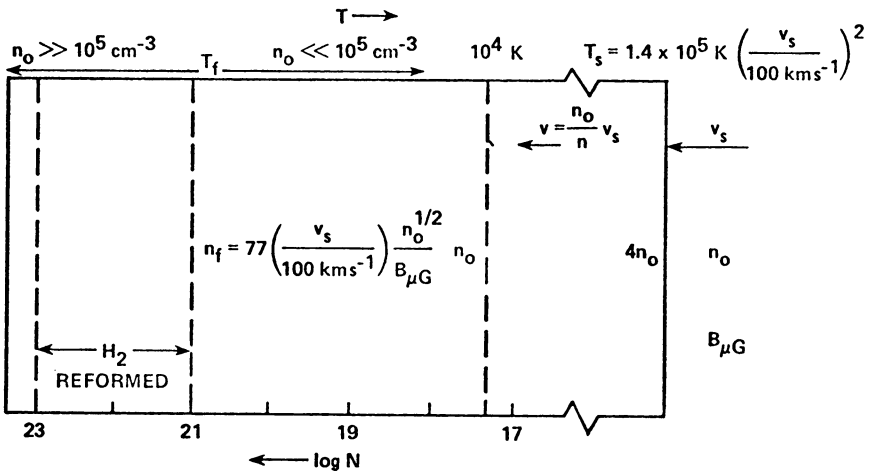


Figure 2. Dissociative shocks ($v_s \gg 30 \text{ km s}^{-1}$)

Slow, non-dissociative shocks initially heat the ambient gas to temperatures $T_s \lesssim 10^{4.5}$ K. For low ambient densities ($n_0 \lesssim 100 \text{ cm}^{-3}$, mainly atomic) the gas rapidly cools to $T < 100$ K by H_2 rotational-vibrational transitions and the 63 μ OI line in a column density $N_h \sim 10^{19} \text{ cm}^{-2}$. Elitzur and Watson (1978) point to the only observational consequence of the hot postshock gas: CH^+ may be produced with sufficient column density $N(\text{CH}^+) \sim 10^{13} \text{ cm}^{-2}$ to explain the relatively high amounts of CH^+ seen in absorption toward early-type stars. Hollenbach, Chu, and McCray (1976), show that H_2 may be formed in the dense, cool ($T < 100$ K), wind-driven postshock gas with rotational populations like those observed by Copernicus toward early-type stars.

For high ambient densities ($n_0 \sim 1000 \text{ cm}^{-3}$, mainly molecular) the $T \sim 1000 \text{ K}$ postshock molecular gas temperatures initiate the chemical reactions to be discussed in the next section; cooling proceeds via molecular rotational and vibrational transitions. Several authors (Hollenbach and Shull 1977, Kwan 1977, London, McCray and Chu 1977) explain the observed H_2 2μ $1-0$ vibrational transitions in Orion as arising behind such shocked gas. In their calculations, which assumed that H_2 dominated the cooling to $T \sim 1000 \text{ K}$, the cooling column density N_{1000} to 1000 K was of order

$$N_{1000} \sim 2 \times 10^{13} n_0 \text{ cm}^{-2} \quad (3)$$

for $n_0 \sim 10^5 \text{ cm}^{-3}$. To explain the H_2 2μ intensity from Orion, $n_0 \sim 10^7 \text{ cm}^{-3}$ is required.

Table 1
Important Chemical Reactions in Hot Neutral Gas

Reaction	Rate Coefficient ($\text{cm}^{-3}\text{s}^{-1}$)	(1)
$\text{H}_2 + \text{O} \rightleftharpoons \text{OH} + \text{H}$	$3 \times 10^{-11} T_3 \exp(-4.48/T_3)$	(2)
	$1.4 \times 10^{-11} T_3 \exp(-3.5/T_3)$	(2)
$\text{Si} + \text{OH} \rightleftharpoons \text{SiO} + \text{H}$	3×10^{-11}	(3)
	$3 \times 10^{-11} \exp(-39.5/T_3)$	(3)
$\text{H}_2 + \text{OH} \rightleftharpoons \text{H}_2\text{O} + \text{H}$	$3.6 \times 10^{-11} \exp(-2.59/T_3)$	(2)
	$1.5 \times 10^{-10} \exp(-10.25/T_3)$	(2)
$\text{H}_2 + \text{C} \rightleftharpoons \text{CH} + \text{H}$	$2.1 \times 10^{-9} T_3^{1/2} \exp(-14.10/T_3)$	(2)
	$2.1 \times 10^{-9} T_3^{1/2} \exp(-2.2/T_3)$	(2)
$\text{H}_2 + \text{C}^+ \rightleftharpoons \text{CH}^+ + \text{H}$	$4.2 \times 10^{-11} T_3^{5/4} \exp(-4.64/T_3)$	(4)
	$4.2 \times 10^{-11} T_3^{5/4}$	(4)
$\text{H}_2 + \text{S} \rightleftharpoons \text{HS} + \text{H}$	$3 \times 10^{-11} \exp(-10.0/T_3)$	(3)
	3×10^{-11}	(3)
$\text{HS} + \text{CO} \rightleftharpoons \text{OCS} + \text{H}$	$3 \times 10^{-11} \exp(-5.36/T_3)$	(3)
	3×10^{-11}	(3)

(1) $T_3 = T/1000 \text{ K}$, lower rate coefficient for reverse reaction;
 (2) Iglesias and Silk (1978); (3) Estimated from Lada, Oppenheimer and Hartquist (1978); (4) Solomon and Klemperer (1972).

3.3 Hot chemistry

High temperature ($T \sim 10^3$ to 10^4 K) neutral gas exists behind both slow and fast shocks. The major high temperature gas phase reactions associated with such regions are listed in Table 1, along with their rate coefficients. These reactions, initiated by H_2 , proceed rapidly because the rate coefficients are high and because the reactants are generally plentiful. Hence, relatively large quantities of OH, H_2O , SiO, HS, OCS, CH, and CH^+ are produced in the hot postshock gas if H_2 is present. Behind fast dissociative shocks, molecular hydrogen formation must proceed before this "hot chemistry" can commence. Hollenbach and McKee (1979a) have shown that production of H_2 occurs primarily on grain surfaces as long as the grain temperatures are less than about 100 K. Grains are warmed by the radiation (energy flux $\propto n_O v_s^3$) from the cooling postshock gas and the grain temperature condition for molecular hydrogen formation reduces to

$$n_O v_s^3 \lesssim 3 \times 10^3 \text{ cm}^{-3} \quad N \lesssim 10^{20} \text{ cm}^{-2} \quad (4)$$

$$n_O v_s^3 \lesssim 2 \times 10^6 \text{ cm}^{-3} \quad N \gtrsim 10^{21} \text{ cm}^{-2}$$

for 0.1μ silicate or graphite grains. The production of H_2 by the H^- process also produces a small fraction ($x(H_2) \lesssim 10^{-3}$) of H_2 in the hot recombing postshock gas (Hollenbach and McKee 1979b).

3.4 Molecular cooling behind shocks

Behind both slow and fast shocks the cooling in the hot neutral regions will be dominated by molecular vibrational-rotational transitions if the gas is substantially molecular. As discussed in Section 3.2, early work focussed on H_2 cooling behind slow shocks, although Kwan (1977) included CO cooling as well. However, Hollenbach and McKee (1979a) have shown that OH and H_2O dominate the cooling when the postshock density exceeds about 10^5 cm^{-3} in warm molecular gas with solar abundances. This result is due, first of all, to the high fractional abundances ($x(OH) \sim x(H_2O) \sim 10^{-4}$) of OH and H_2O in hot molecular gas. Secondly, densities exceeding 10^5 cm^{-3} collisionally quench CO and H_2 relative to OH and H_2O .

4. APPLICATIONS

Recently, the vibrationally and rotationally excited H_2 in Orion has been observed to have high velocity dispersions (FWHM $\sim 50 \text{ km s}^{-1}$) (e.g., Nadeau and Geballe 1979, Beck, Geballe and Lacy 1979). The high preshock densities ($n_O \sim 10^7 \text{ cm}^{-3}$) probably rule out non-dissociative ($v_s \sim 25\text{--}50 \text{ km s}^{-1}$) shocks. Furthermore, high velocity non-dissociative shocks will produce more 2-1 S(1) H_2 line intensity than is observed (Shull and Hollenbach 1978). Therefore, we are led to postulate: (i), slow ($v_s \sim 10 \text{ km s}^{-1}$) shocks traversing clumps of gas with velocity

dispersions of order 50 km s^{-1} , or (ii), dissociative shocks with $v_s \sim 50 \text{ km s}^{-1}$ with H_2 being reformed at high ($T \sim 2000 \text{ K}$) temperatures. The cooling by OH will be important in the second case; preliminary calculations indicate probable fluxes of order $10^{-17} \text{ watts cm}^{-2}$ from far infrared OH rotational transitions. These fluxes are within present detection capabilities (Hollenbach and McKee 1979b).

The observation of accelerated HI, OH, and CO (DeNoyer 1978, 1979a, 1979b, and Giovanelli and Haynes 1979) as well as vibrationally excited H_2 (Treffers 1979) in IC443 has led to a picture of shock waves of velocity $v_s \sim 10$ to 100 km s^{-1} incident upon gas of density $10^2 - 10^3 \text{ cm}^{-3}$. The H_2 probes the hot postshock gas in the non-dissociative shocks while the HI, CO and OH radio observations measure the cold, accelerated, postshock material. Calculations by Hollenbach and McKee (1979b) suggest that the high OH abundance in the hot postshock gas rapidly declines as the gas cools. Therefore, the high observed abundance of cold OH may be an indication of unusual conditions in the cold gas, e.g., a high ionization rate by soft X-rays from the supernova interior.

Finally, as a future application, we note that the simultaneous observation of infrared lines from, for example, H_2 , CI, CO, CII, OI, OH, and H_2O in the hot molecular gas near KL and BN will provide, for the first time, a measure of the H:C:O ratio in a dense molecular cloud.

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DISCUSSION FOLLOWING HOLLENBACH

Field: The rate of reaction of $H_2(v=1)$ with OH has recently been measured to be about 300 times faster than with $H_2(v=0)$. Behind the shock the temperature is sufficiently high that a significant proportion of $H_2(v=1)$ may be available to react rapidly with OH. This may well influence your chemical modelling.

Hollenbach: It would be very interesting to know whether the reaction of H_2 with O behaves similarly. Both these reactions of vibrationally excited H_2 will affect the chemistry for gas with $n \gtrsim 10^6 \text{ cm}^{-3}$ and $T \gtrsim 1000 \text{ K}$.

Slysh: What time is needed for OH to cool from a high "shocked" temperature to the cold, $\sim 100\text{K}$, post-shock temperature?

Hollenbach: The time is approximately 300 years for a 10 km s^{-1} shock incident upon a 10^3 cm^{-3} cloud. The time is inversely proportional to the shock velocity and cloud density, for densities up to about 10^4 cm^{-3} .

Carruthers: Has the (2-1) vibrational H_2 transition been observed toward IC 443? If so, what temperature has been inferred from a comparison with the (1-0) transition?

Hollenbach: It has not yet been observed, but is currently being looked for. If the shock is a 40 km s^{-1} non-dissociative one, we expect the 2-1S(1) line to be almost as intense as the 1-0S(1) line.

Chaffee: Could the A-X OH lines be observed in absorption against a continuum source through the shocks you describe? That is, does the increase in OH production by 10^4 more than offset the increased excitation?

Hollenbach: The OH will be similar to H_2O and CH^+ ; column densities of 10^{12} cm^{-2} to 10^{13} cm^{-2} , most of which is in the ground rotational state because of rapid radiative decays, will be present for shocks incident upon low ($n < 10^3 \text{ cm}^{-3}$) density gas.

Zuckerman: Rickard, Palmer and myself have observed OH in Orion with the Bonn telescope (to be submitted to Ap. J.). The beam was 2.6 arcmin, i.e. not much larger than the high velocity source in Orion. We saw no evidence of wide OH lines even at low levels of intensity.

Elitzur: The OH/ H_2O ratio behind a shock varies with the H_2/H ratio.

The oxygen will be channelled into water and not into OH if the shock runs into dense clouds where the hydrogen is essentially molecular.

Hollenbach: Yes, an absence of hot OH in the KL-BN region would imply that the gas has a high H_2/H ratio. Then if shocks were present, they would be slow non-dissociative shocks as opposed to fast dissociative shocks followed by re-association of H_2 in the hot post-shock gas.

Wootten: I offer observational support of your suggestion of enhanced ionization in cool material between the interior of a supernova remnant and the shock in the surrounding molecular cloud. In the cloud near the W28 remnant there is a small region of very broad HCO^+ emission. At the velocity of the most blueshifted components of HCO^+ the only other molecular emission detected is OH. My study of the HCO^+ indicated that the ionization, in the region in which the blueshifted emission originates, must be enhanced compared to unshocked parts of the cloud. Perhaps, as you suggest for IC443, oxygen charge exchange in this region produces the OH responsible for emission at the most blueshifted velocity.

Drapatz: To compare with the CO surveys one would like a survey of cold dense matter using the S(0) or S(A) rotational transition of H_2 at 28 μm and 17 μm respectively. While pure thermal emission in these lines is undetectably small for clouds of $T \sim 10K$, shock waves due to cloud-cloud collisions, even for small shock velocities, seem to produce detectable effects ($N(H_2) \gtrsim 10^{21} cm^{-2}$, $T \gtrsim 100K$) Has such a model already been worked out?

Hollenbach: Not to my knowledge. To produce $N(H_2) \gtrsim 10^{21} cm^{-2}$ at $T > 100K$ would require a shock of speed $V_s \gtrsim 3 km s^{-1}$ penetrating a rather dense region. The exact density would have to be worked out, but I suspect it may be as high as $10^6 cm^{-3}$.

W. Watson: Why is it clear that the IR emission from H_2 is caused by shocks rather than pumping by ultraviolet radiation? Line widths cannot be used since you are now attributing them to multiple components of the gas.

Hollenbach: It is true that far-UV radiation ($\lambda \sim 100 \text{ \AA}$) can excite the $2\mu H_2$ lines by electronic excitation followed by cascade through the vibrational levels. Two basic questions must be asked about each H_2 source to determine whether this mechanism is important: (i) is the far-UV intensity sufficient and (ii) if more than one line is observed, does the far-UV pump produce the relative strengths of the lines? There is also the problem that, as the far-UV intensity increases and the population of vibrationally-excited H_2 increases, the H_2 can be ionized and destroyed by far-UV photons. Shull has examined this problem and obtains an upper limit to the possible 2μ intensity. All of these arguments show that the H_2 in Orion cannot be pumped by far-UV radiation.