Quantum molecular dynamics simulations of the thermophysical properties of shocked liquid ammonia for pressures up to 1.3 TPa

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Abstract

We investigate via quantum molecular-dynamics simulations the thermophysical properties of shocked liquid ammonia up to the pressure 1.3 TPa and temperature 120000 K. The principal Hugoniot is predicted from wide-range equation of state, which agrees well with available experimental measurements up to 64 GPa. Our systematic study of the structural properties demonstrates that liquid ammonia undergoes a gradual phase transition along the Hugoniot. At about 4800 K, the system transforms into a metallic, complex mixture state consisting of NH$_3$, N$_2$, H$_2$, N, and H. Furthermore, we discuss the implications for the interiors of Uranus and Neptune.

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I. INTRODUCTION

Ammonia, together with water and methane, are the major constituents of the giant planets in our solar system. In particular, Uranus and Neptune are thought to have “hot ice” layers predominantly made up of 56% water, 36% methane, and 8% ammonia in proportions \[1, 2\]. The behavior of these molecular compounds at extreme conditions (temperatures \(T > 2000\) K, pressures \(P > 20\) GPa) is therefore crucial for understanding Uranus and Neptune physics, including gravitational moments, atmospheric composition, and magnetic field \[3\]. As a weakly hydrogen-bonded liquid, the thermophysical properties of ammonia at high pressure and high temperature are of fundamental interest both for astrophysics and solid state physics.

Experimental researches on ammonia are indispensable for exploring its characteristics under extreme conditions. Standard explosive techniques were firstly used to get the Hugoniot curve of ammonia up to 39 GPa. In this pressure region, no transition was observed along the Hugoniot \[4\]. Mitchell \textit{et al.} have used two-stage light-gas gun to reach pressure of 64 GPa \[5\]. The first shock temperature measurements on ammonia were performed at pressures of 61 and 48 GPa for diagnosing the physics occurring at these extreme conditions \[6\]. Through comparing with the calculations using fluid perturbation theory \[7\], it was concluded that there may exist absorption mechanism at these high pressures. Previous electrical conductivity measurements have shown that ammonia becomes conductive in the pressure range of 7-28 GPa \[8, 9\], which is thought to be induced by molecular dissociation-ionization. Several static experimental studies performed in diamond anvil cells were limited to the phase diagram up to 60 GPa and 2500 K \[10–12\].

On theoretical side, ammonia has been predicted to become a protonic conductor above 60 GPa and 1200 K using \textit{ab initio} molecular dynamics \[13\]. At even more extreme conditions, ammonia molecules are expected to dissociate and react at very rapid rates \[13, 14\]. In addition, first-principles calculations have shown that driven by the entropy of mixing term in the free energy formulation \[12\], ammonia molecules chemically dissociate to \(\text{N}_2\) and \(\text{H}_2\) above approximately 7 GPa and 900 K.

In this paper, we perform the first comprehensive quantum molecular dynamics (QMD) simulations of the high-pressure and high-temperature behavior of ammonia with densities and temperatures ranging from 0.7 g/cm\(^3\) and 230 K to 2.6 g/cm\(^3\) and 120000 K along the
principal Hugoniot. We determine the equation of state (EOS) in the warm dense region by means of QMD, where the active electrons are treated in a full quantum mechanical way within the finite-temperature density functional theory (FT-DFT). This method has been proven to be a successful tool to calculate physical properties of complex plasmas under such extreme conditions [15–20]. In combination with the Kubo-Greenwood formulation, we derive the electrical and optical properties in order to locate the nonmetal-to-metal transition. Through analyzing the concentration of molecular species along the Hugoniot based on pair correlation function, we explore and describe the mechanism for this transition.

II. COMPUTATIONAL METHOD

A. Quantum molecular dynamics

The particular implementation of QMD method used in the present study comes from the Vienna ab initio simulation package (VASP) plane-wave pseudopotential code developed at the Technical University of Vienna [21, 22], in the framework of a FT-DFT [23, 24]. The electronic states are populated according to the Fermi-Dirac statistics, with electronic temperature set equal to that of ions. We consider the electronic states occupied down to $10^{-6}$. The electron wavefunctions are calculated using the all-electron projector augmented wave (PAW) potentials [25, 26]. The Perdew-Wang 91 parametrization of the generalized gradient approximation (GGA) [27] is employed for the exchange-correlation energy. Atoms move classically according to the forces, which originate from the interactions of ions and electrons.

QMD simulations are performed in the canonical (NVT) ensemble with Nose-Hoover thermostat for selected densities from 0.7 to 2.6 g/cm$^3$ and temperatures from 230 to 120000 K that highlight the single-shock Hugoniot region. 27 nitrogen and 81 hydrogen atoms (twenty-seven ammonia molecules) are treated in a cubic cell of the size appropriate to the considered density. We fix the plane-wave cutoff at 550.0 eV which is tested to give good convergence for both total energy and pressure. The Brillouin zone sampling of 108-atom calculations use only the $\Gamma$ point for molecular dynamics, while $4 \times 4 \times 4$ Monkhorst-Pack [28] scheme $k$ points for the calculations of electronic properties. Integration of the equations of motion proceed with time step of 0.5-1.0 fs for different pressure-temperature ranges. After
about 3 ps the system is equilibrated and the subsequent 5 ps are taken to calculate the EOS and electronic properties as running averages. The ion temperature $T_i$ is fixed using velocity scaling, while the electron temperature $T_e$ is in turn set to that of the ions $T_i$ based on the assumption of local thermodynamical equilibrium.

B. Optical properties

At the Hugoniot points the electronic properties are calculated for ten configurations selected from an equilibrated (in an average sense) portion of the molecular dynamics run. The configurations are spaced at time steps separated by at least the correlation time, the $e$–folding time of the velocity autocorrelation function. For each of these configurations, the Kubo-Greenwood formulation is used to calculate the electrical conductivity, without particular assumptions made on the ionic structure or on the electron-ion interactions. In the framework of the quasi-independent particle approximation, the Kubo-Greenwood formulation $^{[29, 30]}$ gives the real part of the electrical conductivity as a function of frequency $\omega$,

$$\sigma_1(\omega) = \frac{2\pi}{3\omega\Omega} \sum_k w(k) \sum_{j=1}^N \sum_{i=1}^N \sum_{\alpha=1}^3 \left[ f(\epsilon_i, k) - f(\epsilon_j, k) \right]$$

$$\times |\langle \Psi_{j,k} | \nabla_\alpha |\Psi_{i,k} \rangle|^2 \delta(\epsilon_j, k - \epsilon_i, k - \hbar\omega),$$  

(1)

where $\omega$ is the frequency, $\Omega$ is the atomic volume, and $N$ is the total number of bands used. $\Psi_{i,k}$ and $\epsilon_{i,k}$ are the electronic eigenstate and eigenvalue for the electronic state $i$ at $k$, $f(\epsilon_i, k)$ stands for the Fermi distribution function, and $w(k)$ represents the $k$–point weighting factor. Other properties can be directly derived from the frequency-dependent real part of the electrical conductivity. The imaginary part $\sigma_2(\omega)$ is obtained by using the Kramer-Krönig relation

$$\sigma_2(\omega) = -\frac{2}{\pi} P \int \frac{\sigma_1(\nu) \omega}{(\nu^2 - \omega^2)} d\nu,$$

(2)

where $P$ denotes the principal value of the integral. The complex dielectric function, in turn, follows immediately from the complex conductivity,

$$\epsilon_1(\omega) = 1 - \frac{4\pi}{\omega} \sigma_2(\omega),$$

(3)
\[ \epsilon_2 (\omega) = \frac{4\pi}{\omega} \sigma_1 (\omega). \] (4)

And then the real \( n (\omega) \) and imaginary \( k (\omega) \) parts of the index of refraction have a relation with the complex dielectric function by a simple formula,

\[ \epsilon (\omega) = \epsilon_1 (\omega) + i\epsilon_2 (\omega) = [n (\omega) + ik (\omega)]^2. \] (5)

Finally, the reflectivity \( r (\omega) \) and absorption coefficient \( \alpha (\omega) \) can be determined from these quantities as follows

\[ r (\omega) = \frac{[1 - n (\omega)]^2 + k (\omega)^2}{[1 + n (\omega)]^2 + k (\omega)^2}, \] (6)

\[ \alpha (\omega) = \frac{4\pi}{n (\omega) c} \sigma_1 (\omega). \] (7)

III. RESULTS AND DISCUSSIONS

A. Hugoniot

As a crucial measure for theoretical EOS data, the Hugoniot describes the locus of states satisfying the Rankine-Hugoniot equation \([31]\), which follows from the conservation of mass momentum and energy across the shock front. The initial and final internal energy, pressure and volume, respectively, \( (E_0, P_0, V_0) \) and \( (E, P, V) \) are related through such an equation in the form

\[ (E_1 - E_0) + \frac{1}{2} (V_0 - V_1) (P_0 + P_1) = 0, \] (8)

where the internal energy \( E \) equals to the sum of the ion kinetic energy \( \frac{3}{2} k_B T_i \), the time average of the DFT potential energy, and zero-point energy. The pressure consists of contributions from the electronic \( P_e \) and ionic \( P_i \) components, which come from, respectively, the derivatives taken with respect to the Kohn-Sham electronic orbitals and the ideal gas expression since ions move classically. We thus have \( P = P_e + \rho_n k_B T \), where \( \rho_n \) is the
TABLE I: Points along the principal ammonia Hugoniot derived from DFT-MD simulations at a series of density ($\rho$), pressure ($P$), and temperature ($T$).

| $\rho$ ($\text{g/cm}^3$) | $P$ (GPa) | $T$ (K) | $U_p$ (Km/S) | $U_s$ (Km/S) |
|---------------------------|-----------|---------|---------------|---------------|
| 0.80                      | 1.24      | 250     | 0.487         | 3.655         |
| 1.00                      | 3.73      | 308     | 1.284         | 4.186         |
| 1.2                       | 14.33     | 1735    | 2.955         | 6.998         |
| 1.4                       | 25.41     | 2295    | 4.301         | 8.521         |
| 1.6                       | 41.43     | 3082    | 5.820         | 10.269        |
| 1.7                       | 51.53     | 3562    | 6.634         | 11.203        |
| 1.8                       | 63.28     | 4174    | 7.491         | 12.184        |
| 1.9                       | 77.09     | 4791    | 8.404         | 13.232        |
| 2.0                       | 95.94     | 6036    | 9.509         | 14.554        |
| 2.2                       | 221.44    | 19180   | 14.790        | 21.595        |
| 2.4                       | 567.67    | 54229   | 24.130        | 33.932        |
| 2.6                       | 1273.65   | 112663  | 36.705        | 50.051        |

number density. The particle velocity of material behind the shock front $u_p$ and the shock velocity $u_s$ are then determined from the other two Rankine-Hugoniot equations [31],

$$V_1 = V_0 \left[1 - (u_p/u_s)\right],$$  \hspace{1cm} (9)

$$P_1 - P_0 = \rho_0 u_s u_p.$$ \hspace{1cm} (10)

In the present work, the initial internal energy of ammonia is calculated to be $E_0 = -18.64$ eV/molecule under the experimental condition with $\rho_0 = 0.6933 \text{ g/cm}^3$ at a temperature of 230 K. The initial pressure can be neglected when compared to the high pressure of shocked state along the Hugoniot. To find the Hugoniot points for a given $V_1$, a series of simulations are performed for different temperatures $T$. $E_1$ and $P_1$ are then fitted to a cubic function of $T$. We plot $(E_1 - E_0)$ and $\frac{1}{2} (V_0 - V_1) (P_0 + P_1)$ as a function of $T$, and the intersection fixes the point satisfying Eq. (8). The principal Hugoniot points of ammonia derived from Rankine-Hugoniot equations are listed in Table I.
FIG. 1: Principal Hugoniot of liquid ammonia. For comparison, previous experimental data (Ref. 4, Ref. 5, Ref. 6 and Ref. 9) and theoretical results along planetary isentrope (Ref. 13) are also included.

Figure 1 shows the pressure and temperature as functions of density along the Hugoniot curve for ammonia, along with experimental measurements and results from previous ab initio molecular dynamic simulations along the planetary isentrope for comparison. We find a very good agreement with the experimental results all along the single-shock Hugoniot up to 64 GPa, while we also predict the behavior of ammonia under higher pressures and temperatures, which may be testified in future experiments. The data along the planetary isentrope of Ref. 13 presents a prominent discrepancy with our QMD results, which is because that the temperature along the planetary isentrope is different from the shock temperature. In addition, the Hugoniot curve is naturally divided into three segments with their respective features, similar to hot dense methane [32]. The temperature is found to increase linearly with density up to 2000 K, which results from the fact that ammonia remains its ideal molecular configurations without dissociation. In the temperature range of 2000-6000 K, a plateau appears and the temperature no longer increases as rapidly as the corresponding
density. As discussed in more detail later, this region coincides with the onset of a significant fraction of molecular dissociation and the transformation to a complex mixture consisting of a variety of species, including NH₃, H₂, N₂, H, and N. Furthermore, it will be reported that ammonia becomes metallic at these temperature-pressure conditions. Beyond 6000 K the temperature increases rapidly with density again with the slope depending on the initial density. In this regime, some ionic species exist with very short lifetime and the system enters into a plasma state.

The Hugoniot curves for several other initial densities and temperatures are also presented in Fig. 2 in order to explore different pressure-temperature conditions of interest to future experimental measurements. It can be seen that subtle changes in the starting density allow liquid ammonia to reach different regions of the pressure and temperature, while the moderate variations in the initial temperature do not. It is highly desirable as a means for one to understand the properties of liquid ammonia over a wide range of extreme conditions. These predicted Hugoniots may be verified by utilizing modern experimental approaches.

We further plot temperature as a function of pressure along each of the Hugoniot curves with different initial densities in Fig. 3, in which the isentropes for Uranus and Neptune are also included [33]. At approximately 2000-6000 K, with ammonia entering into complex mixture state, the slopes change obviously. As can be seen from Fig. 3, the isentropes intersect these Hugoniot curves just in this region. It implies that ammonia does not remain its ideal molecular form in the interiors of Uranus and Neptune, but transforms into a mixture of NH₃, H₂, N₂, H, and N. In addition, the phase diagram of ammonia determined by Cavazzoni et al. [13] has shown that a superionic phase exists far below the isentropes of Uranus and Neptune. And thus it could be predicted that molecular hydrogen may be expelled from the interiors of Uranus and Neptune into the outer layer. The cores of these planets may become more compact.

B. Liquid structure

To quantify the structural change in ammonia along the Hugoniot, we calculate the pair-correlation function for each possible species of NH₃, N₂, and H₂. The pair-correlation function gives the possibility of finding an atom of a given type at a given distance from a reference atom. The results are presented in Fig. 4. At the lowest density $\rho = 0.6933 \text{ g/cm}^3$, 
FIG. 2: $P - \rho$ and $T - \rho$ Hugoniot curves computed for several initial conditions.

FIG. 3: Temperature as a function of pressure along the shock Hugoniot curves from Fig. 2 for different initial densities. The isentropes for Uranus and Neptune are also included.
FIG. 4: Pair-correlation functions for N-N (black line), N-H (blue line), H-H (red line) along the principal ammonia Hugoniot. (a) $\rho = 0.6933 \, g/cm^3$, $T = 230 \, K$; (b) $\rho = 1.6 \, g/cm^3$, $T = 3082 \, K$; (c) $\rho = 1.8 \, g/cm^3$, $T = 4174 \, K$; (d) $\rho = 2.0 \, g/cm^3$, $T = 6036 \, K$; (e) $\rho = 2.2 \, g/cm^3$, $T = 19180 \, K$; (f) $\rho = 2.4 \, g/cm^3$, $T = 54229 \, K$.

the sharp peak at about 1.02 Å corresponding to the equilibrium internuclear distance of the N-H bond in ammonia molecule and the following minimum close to zero indicate that ammonia remains its ideal molecular configurations stably. As the density is raised to $\rho=1.6$ g/cm$^3$, new N-N peak begins to emerge at the equilibrium distance of nitrogen molecule 1.2 Å. Meanwhile, the maxima of $g_{N-H}(r)$ are reduced and broadened significantly. It is indicated that ammonia molecules dissociate and small amount of nitrogen molecules form at this density. At 1.8 g/cm$^3$, N-H peak continues to be reduced and broadened while the peaks of N-N and H-H increase. This trend persists up to a density of 2.0 g/cm$^3$. With increasing the density further, the N-H peak diminishes, while N-N and H-H peaks are broadened and even flattened. This suggests that all molecules are very short-lived and unstable at these extreme conditions.

C. Dynamic optical and electronic properties

Using the Kubo-Greenwood formula, we calculate the real part of frequency-dependent conductivity $\sigma_1(\omega)$ for points along the Hugoniot (with the initial condition $\rho_0=0.6933$
FIG. 5: The real part of electrical conductivity $\sigma_1(\omega)$ along the principal Hugoniot. Data have been averaged over 10 uncorrelated MD configurations. (Inset) dc conductivity of our results and experimental data from Ref. 9 are plotted along the principal Hugoniot.

Calculation of $\sigma_1(\omega)$ given by Eq. (1) typically involves 1000 states, which insures adequate convergence over the frequency range we considered. The maximum of $\sigma_1(\omega)$ around 10 eV can be attributed to the transitions to the lowest excited states. It is found that the peak moves to lower frequency with increasing density and temperature, and thus leads to a significant increase in dc conductivity, which is defined as $\sigma_{dc} = \lim_{\omega \to 0} \sigma_1(\omega)$. The significant variation of the dc conductivity along the principal Hugoniot is highlighted in Fig. 5 as an inset. We first notice that the dc conductivity becomes nonzero when approaching 50 GPa. For pressures below 65 GPa, our calculated dc conductivity agrees well with the attainable experimental data. After that, the dc conductivity rises rapidly to a value larger than 1000 $\Omega^{-1}\text{cm}^{-1}$ for pressures between 65 and 75 GPa. Based on the definition of metallicity of the disordered system which has been discussed for warm dense methane [34], it could be concluded that nonmetal-metal transition takes place in shocked ammonia. Then, a plateau is reached near 220 GPa, which has been observed in some other molecular fluids [35, 36]. Such a behavior of the dc conductivity can be ascribed to the dissociation of the molecules as discussed below.

To clarify the nature of the fluid along the Hugoniot, we present in Fig. 6(a) the variation of the dissociation fraction of ammonia molecules as a function of density. Following the
QMD simulations, we identify ammonia molecules from the trajectories based on a simple bond-length criteria. A cutoff radius of 1.25 Å is used to construct a sphere about each nitrogen atom and all hydrogen atoms within this region are considered as bound to this reference nitrogen atom. The number of ammonia molecules is counted at each configuration and then averaged along the trajectory. As seen from Fig. 6(a), the fluid has been partially dissociated at 1.7 g/cm$^3$. Whereas, at 2.2 g/cm$^3$ and above, the system is fully dissociated. Similarly, from the conductivity curve shown in Fig. 6(b), we can find that the variation of dc conductivity as a function of density closely follows the variation of molecular dissociation fraction. This intimate connection suggests that dissociation has important influence on the electrical properties of the system and results in the nonmetal-metal transition consequently.

In dynamic shock compression experiments, optical reflectivity is one of the readily observables. For ammonia, we show in Fig. 7(a) the variation of the dynamic reflectivity $r(\omega)$ along the Hugoniot. With the increase of the density and temperature, the shape of the curve changes abruptly at 1.9 g/cm$^3$, which is related with the high-pressure nonmetal-metal transition. Correspondingly, the reflectivity at typical wavelengths of 350 and 720 nm increases sharply around 75 GPa, as shown in Fig. 7(b). Furthermore, the increase in reflectivity mostly ceases and reaches a plateau near 220 GPa where ammonia molecular are fully dissociated. It can be seen that a measurable reflectivity increase from 0.02 to 0.5-0.6 arises for the principal shocks.
(a) Reflectivity at wavelengths of 7200 (black square) and 3500 Å (red circle) as a function of pressure along the Hugoniot.

(b) Density of states (DOS) for liquid ammonia along the principal Hugoniot: (a) \( \rho = 1.4 \text{ g/cm}^3, T = 2295 \text{ K} \); (b) \( \rho = 1.8 \text{ g/cm}^3, T = 4174 \text{ K} \); (c) \( \rho = 2.0 \text{ g/cm}^3, T = 6036 \text{ K} \); (d) \( \rho = 2.2 \text{ g/cm}^3, T = 19180 \text{ K} \). Data have been averaged over 10 uncorrelated MD configurations. The zero of the energy scale shows the position of the Fermi level.
One way to characterize the behavior of nonmetal-metal transition is the variation of the electron density of state (EDOS) along the Hugoniot as shown in Fig. 8. It is found that a gap about 2.0 eV appears at $\rho = 1.4 \text{ g/cm}^3$ and $T = 2295 \text{ K}$, with only thermally activated electron transport occurring. With ammonia molecules dissociate, the resulting atoms act as dopants and progressively fill the dense fluid band gap, and eventually leads to a metal-like behavior.

IV. CONCLUSIONS

In conclusion, we have predicted the Hugoniot of ammonia up to 1.3 TPa, which is in good agreement with available shock experiments with pressure up to 64 GPa. For comparison with future experiments, we have also computed several Hugoniot curves with different initial states. Three characterized segments are identified along the Hugoniot. As the system dissociates and transforms into complex mixture state, nonmetal-metal transition takes place, which is determined through analyzing the electrical conductivity and optical reflectivity. In addition, the isentropes of Uranus and Neptune pass through the temperature-pressure conditions of the mixture regime along the Hugoniot, while the superionic phase of ammonia exists far below the isentropes. Therefore, we conclude that molecular hydrogen could release into outer layers, which leads to more compact cores in these planets.

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