

Elastic And Kinetic Properties Of Liquid Nitrogen

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ABSTRACT

Molecular dynamic simulation has been applied to study the elastic and kinetic properties of liquid nitrogen such as shear modulus, bulk modulus, shear waves speed, work done by a diffusing particle, pressure and internal energy. An interaction model chosen for this calculation is known as Lennard Jones pair potential. The temperature at which these properties were calculated range from 20k to 81k while the density range from 0.789g/cm³. The calculated properties decrease with the State points except the internal energy of atoms which increase as temperature increases and density deceases. The shear and bulk modulus of solid nitrogen at temperature 20k compared well with experimental values.

Keywords: Elastic And Kinetic Properties Of Liquid Nitrogen

1. INTRODUCTION

Nitrogen is a chemical element with symbol N and atomic number 7. It is the lightest nitrogen and at room temperature, it is a transparent, odourless diatomic gas. Nitrogen is a common element in the universe, estimated at about seventh in total abundance in the Milky Way and the Solar System. On Earth, the element forms about 78% of Earth's atmosphere and is the most abundant un-combined element. The element nitrogen was discovered as a separable component of air by Scottish physician Daniel Rutherford in 1772. Many industrially important compounds, such as ammonia, nitric acid, organic nitrates (propellants and explosives), and cyanides, contain nitrogen. The extremely strong triple bond in elemental nitrogen (N=N) dominates nitrogen chemistry, causing difficulty for both organisms and industry in converting the N₂ into useful compounds, but at the same time causing release of large amounts of often useful energy when the compounds burn, explode, or decay back into nitrogen gas. Synthetically produced ammonia and nitrates are key industrial fertilizers, and fertilizer nitrates are key pollutants in the eutrophication of water systems.

Apart from its use in fertilizers and energy—stores, nitrogen is a constituent of organic compounds as diverse as Kevlar fabric and cyanoacrylate “super” glue. Nitrogen is a constituent of every major pharmacological drug class, including antibiotics. Many drugs are mimics or pro-drugs of natural nitrogen-containing signal molecules: for example, the organic nitrates nitro-glycerin and nitroprusside control blood pressure by metabolizing into nitric oxide. Plant alkaloids (often defence chemicals) contain nitrogen by definition, and many notable nitrogen-containing drugs, such as caffeine and morphine, are either alkaloids or synthetic mimics that act (as many plant alkaloids do) on receptors of animal neurotransmitters (for example, synthetic amphetamines). Nitrogen occurs in all organisms, primarily in amino acids (and thus proteins), in the nucleic acids (DNA and RNA) and in the energy transfer molecule adenosine triphosphate. The human body contains about 3% by mass of nitrogen, the fourth most abundant element in the body

after oxygen, carbon, and hydrogen. The nitrogen cycle describes movement of the element from the air into the biosphere and organic compounds, then back into the atmosphere.

1.1 Properties of Nitrogen

Nitrogen is a non-metal, with an electro negativity of 3.04 . It has five electrons in its outer shell and is, therefore, trivalent in most compounds. The triple bond in molecular nitrogen (N_2) is one of the strongest. The resulting difficulty of converting N_2 into other compounds, and the ease (and associated high energy release) of converting nitrogen compounds into elemental N_2 have dominated the role of nitrogen in both nature and human economic activities.

At atmospheric pressure, molecular nitrogen condenses (liquefies) at 77K ($-195.79\text{ }^\circ\text{C}$) and freezes at 63 K ($-210.01\text{ }^\circ\text{C}$) into the beta hexagonal close-packed crystal allotropic form. Below 35.4 K ($-237\text{M }^\circ\text{C}$) nitrogen assumes the cubic crystal allotropic form (called the alpha phase). Liquid nitrogen, a fluid resembling water in appearance, but with 80.8% of the density (the density of liquid nitrogen at its boiling point is 0.808g/mL), is a common cryogen.

Unstable allotropes of nitrogen consisting of more than two nitrogen atoms have been produced in the laboratory, like N_3 and N_4 . Under extremely high pressures (1.1 million atm) and high temperatures (2000 K), as produced in a diamond anvil cell, nitrogen polymerizes into the single-bonded cubic gauche crystal structure. This structure is similar to that of diamond, and both have extremely strong covalent bonds. N_4 is nicknamed nitrogen diamond. Other (theoretical but not yet synthesized) allotropes include hexazine (N_6 , a benzene analog) and octaazacubane (N_8 , a cubane analog). The former is predicted to be highly unstable, while the latter is predicted to be kinetically stable, by reason of its orbital symmetry.

1.2 Uses of Nitrogen

Nitrogen gas has a variety of applications, including:

- As an inert replacement for air where oxidation is undesirable
- As a modified atmosphere pure or mixed with carbon dioxide, to preserve the freshness of packaged or bulk foods
- In ordinary incandescent light bulbs as an inexpensive alternative to argon
- In production of electron tubes such as transistors, diodes, and integrated circuits
- Filling automotive and aircraft tires due to its inertness and lack of moisture or oxidative qualities, as compared to air
- As a propellant for draft wine, and as an alternative to or in combination with carbon dioxide in carbonated beverages

Nitrogen is also used in preparing samples for chemical analysis to concentrate and reduce the volume of liquid samples. Directing a pressurized stream of nitrogen gas perpendicular to the surface of the liquid allows the solvent to evaporate while leaving the solute(s) and unevaporated solvent behind. Nitrogen tanks are also replacing carbon dioxide as the main power source for paintball guns. But, nitrogen must be kept at higher pressure than CO_2 , making N_2 tanks heavier and more expensive.

1.3 Air balloon submerged in Liquid nitrogen

Liquid nitrogen is a cryogenic liquid. At atmospheric pressure, it boils at $-195.8\text{ }^{\circ}\text{C}$ ($-320.4\text{ }^{\circ}\text{F}$). When insulated in proper containers such as Dewar flasks, it can be transported without much evaporative loss. Like dry ice, the main use of liquid nitrogen is as a refrigerant. Among other things, it is used in the cryopreservation of blood, reproductive cells (sperm and egg), and other biological samples and materials. It is used in the clinical setting in cry therapy to remove cysts and warts on the skin. It is used in cold traps for certain laboratory equipment and to cool infrared detectors or X-ray detectors. It has also been used to cool central processing units and other devices in computers that are over clocked, and that produce more heat than during normal operation.

1.4 Research Motivation

It is widely believed that the shear modulus of a liquid is zero. In fact, this is often taken as a definition of the liquid state. But this is not true. The Born-/Green expression for the shear modulus is well defined (Born, 1939; Born and Huang, 1954 and Green, 1954) and yields non-zero results even for the fluid state (Zwanzig and Mountain, 1965). Zwanzig and Mountain used this expression to calculate the shear and bulk moduli of monoatomic Lennard-Jones fluids such as Helium, Neon, Argon, Krypton and Xenon. It is essential to extend the calculation to diatomic Lennard-Jones fluids such as Nitrogen.

1.5 Objectives of Research

The objectives of this research include the following.

- Calculation of the shear and bulk moduli of nitrogen.
- Determination of shear wave speed.
- Determination of the work done by diffusing particles of nitrogen
- Calculation of pressure and internal energy of nitrogen at different temperatures and densities.

2. LITERATURE REVIEW

2.1 Thermodynamic properties of nitrogen

Armstrong in 1954 measured the vapour pressure of nitrogen in the liquid range below the normal boiling point can be represented by $\log p(\text{mm}) = 6.49594 - 255.82 \log(t-6.600)$. The normal boiling point calculated from this equation is 77.364 K , nitrogen vapour densities along the saturation curve represented by $\log pT^{3.39858} - 282.953 \log(T-3.83)$, the fugacity function in f/p for the saturated vapour is tabulated, this volume covers the thermodynamic properties of gaseous and liquid nitrogen for temperatures between the triple point and 1500 K , and pressures 0.01 to 100 MPa . The authors have analyzed and correlated a vast amount of international experimental data leading to these reliable tables that reflect the thermal properties of this important element. This volume contains: experimental data on thermodynamic properties of nitrogen; methods of deriving the equation of state and calculating thermodynamic tables; the equation of state and evaluation of computed thermodynamic functions relative to experimental data; tables of the thermodynamic properties of nitrogen (Armstrong, 1954). Jacobson, et al., 1988 study a new fundamental equation explicit in Helmholtz energy for thermodynamic properties of nitrogen from the freezing line to 2000 K at pressure to 1000 MPa is presented. New independent equations for the vapour pressure and for the saturated liquid and vapour densities as functions of temperature are also included. The fundamental equation was selected from a comprehensive function of 10.0 terms on the basis of a statistical analysis of the quality of the fit. The coefficients of the fundamental equation were determined by a weighted least-squares fit to selected P - p - T data, saturated liquid and saturated vapour density data to define the phase equilibrium criteria for coexistence, and velocity of sound data.

The fundamental equation and the derivative functions for calculation the internal energy, enthalpy, entropy, isochoric heat capacity (C_v) isobaric heat capacity (C_p) and velocity of sound included. Tables of thermodynamic properties of nitrogen are given for liquid and vapour state within the range of validity of the fundamental equation. The fundamental equation reported here may generally be used to calculate pressures and densities with an uncertainty of $\pm 0.1\%$, heat capacities within $\pm 3\%$, and velocity of sound values within $\pm 3\%$. comparisons of calculated properties experimental data are included to verify the accuracy of the formulation (Jacobson. *et al.*. 988).

Tchouar et al., 2003 carried out the molecular dynamics calculations in order to find the properties of Lennard Jones liquids in different state points of their phase diagram. The spherical shape and the stability of the helium, neon, methane and nitrogen make the liquids easily assessable to numerical simulation. Thermodynamic, structural, and transport properties are studied and compared with both experimental data and recent theoretical investigation In the present work up to 22 state points are covered some of which are near or at the triple point. It will be shown that the classical approach leads to data that are in very good agreement with experiments and other types of calculations. At high temperatures and low densities, we observe a decrease in the uncertainties in the stress autocorrelation function by increasing the number of iterations (Tchouar et al., 2003).

2.2 Transport properties of nitrogen

Millat and wakeham in 1989 presents accurate representation for the thermal conductivity of the diatomic gases nitrogen and carbon monoxide in the limit of zero density. These gases were studied because they have nearly the same molecular mass and viscosities. In contrast, the new analysis confirms that the thermal conductivities of the two gases differ remarkably especially at low temperatures. The theoretically-based correlations provided are valid for the temperature range 220-2100K and have associated uncertainties of $\pm 1\%$ between 300 and about 500K, rising to $\pm 2.5\%$ at the low and high temperature extremes. A comparison with some empirical and semi empirical correlation is given. Transport properties including collective and tracer diffusivities of nitrogen, modeled as a diatomic molecule, in single walled carbon nanotubes have been studied by equilibrium molecular dynamics at different temperatures and as a function of pressure. It is shown that while the asymptotic decay of the translational and rotational velocity autocorrelation function is algebraic, the collective velocity decays exponentially with the relaxation time related to the interfacial friction.

3. METHODOLOGY

3.1 Molecular Dynamic Simulation

molecular dynamics (MD) is a computer simulation method for studying the physical movements of atoms and molecules, and is thus a type of N-body simulation. The atoms and molecules are allowed to interact for a fixed period of time, giving a view of the dynamical evolution of the system. In the most common version, the trajectories of atoms and molecules are determined by numerically solving Newton's equations of motion for a system of interacting particles, where forces between the particles and their potential energies are calculated using inter-atomic potential or molecular mechanics force fields. The method was originally developed within the field of theoretical physics in the late 1950s but is applied today mostly in chemical physics, materials science and the modeling of bio-molecules. Because molecular systems typically consist of a vast number of particles, it is impossible to determine the properties of such complex systems analytically; MD simulation circumvents this problem by using numerical methods. However, long MD simulations are mathematically ill- conditioned, generating cumulative errors in numerical integration that can be minimized with proper selection of algorithms and parameters, but not eliminated entirely.

For systems which obey the ergodic hypothesis, the evolution of a single molecular dynamics simulation may be used to determine macroscopic thermodynamic properties of the system: the time averages of an ergodic system correspond to micro-canonical ensemble averages. MD has also been termed “statistical mechanics by numbers” and “Laplace’s vision of Newtonian machines of predicting the future by animating nature’s forces and allowing insight into molecular motion on an atomic scale.

3.2 Areas of application and limitations

Beginning in theoretical physics, the method of MD gained popularity in materials science and since the 1970s also in biochemistry and biophysics. MD is frequently used to refine three-dimensional structures of proteins and other macromolecules based on experimental constraints from X-ray crystallography or NMR spectroscopy. In physics, MD is used to examine the dynamics of atomic-level phenomena that cannot be observed directly, such as thin film growth and ion-sub-plantation. It is also used to examine the physical properties of nano-technological devices that have not been or cannot yet be created. In biophysics and structural biology, the method is frequently applied to study the motions of biological macromolecules such as proteins and nucleic acids, which can be useful for interpreting the results of certain biophysical experiments and for modeling interactions with other molecules, as in ligand docking. The results of MD simulations can be tested through comparison to experiments that measure molecular dynamics, of which a popular method is nuclear magnetic resonance spectroscopy. MD-derived structure predictions can be tested through community-wide experiments in protein structure prediction, although the method has historically had limited success in this area. Michael Levitt, who shared the Nobel Prize awarded in part for the application of MD to proteins, wrote in 1999 that CASP participants usually did not use the method due to “a central embarrassment of molecular mechanics, namely that energy minimization or molecular dynamic generally leads to a model that is less like the experimental structure” Improvements in computational resources permitting more and longer MD trajectories to be calculated, combined with modern improvements in the quality of force field parameters, have yielded some improvements in performance of both structure prediction and homology model refinement, without reaching the point of practical utility in these areas; most such work identifies force field parameters as a key area for further development.

3.3 Steps Involved In Molecular Simulations

Selection of a potential model

The term r^{-12} dominating at short distance models the repulsion between atoms when they are brought very close to each other. The term r^{-6} dominating at large distance is an attractive term that arises from the weak, long range forces (or Van Der Waals forces). These attractive forces bind the atoms together at long range. The attractive forces play only a minor role in determining the structure of fluids (Hansen and McDonald, 1986). The effect of the attractive term is removed by introducing a cut off radius, r_c . The potential function is neglected beyond r_c and time potential function is calculated as E_{cut} and added to the potential function. The resulting cut and smoothed’ potential then will be given thus:

Where
$$U(r_{ij}) = 4 \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^6 \right] - E_{cut}$$

The total potential of a system of a containing many atoms is given as

$$V(r_i) = \frac{1}{2} \sum_i U(r_i)$$

The summation is a double summation over all atoms; the factor is included to avoid overcrowding of the atoms.

Evans and Morris, 1990 describes a potential inter-atomic interaction among particles in a system of many particles. Rare gases exhibit simple inter-atomic interaction so that the description of the interactions by the Lennard Jones potential is sufficient. The LJ potential is given by:

$$U(r_{ij}) = 4\epsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^{12} - \left(\frac{\sigma}{r_{ij}} \right)^6 \right]$$

Where σ is the diameter, ϵ is the U energy parameter and r_{ij} inter-atomic distance between atoms I and J.

Computation of Potential and forces on all atoms

On all atoms the potential and forces must be calculated. It will have to do with the force exerted by atom j on i.

For a system of N atoms interacting with LJ potential, $U(r_{ij})$ the Force F_i , exerted on atom I is given as;

$$F_i = -\frac{dU(r_{ij})}{dr_{ij}}$$

3.4 Integration of the equation of motion

MD method is deterministic; once the positions and velocities of atom are known, the state of the system can be predicted at any time in the future or the past. From these trajectories the average values of properties are determined.

The MD simulations method based on Newton's law of motion, $F_i = m_i a_i$ where F_i the force is exerted on a particle I, m_i is its mass and a_i is the acceleration. Integration of the equation of motion yields trajectory that describes the positions, velocities and acceleration of the particles as they vary with time, Newton's equation of motion for atom I is given as;

$$F_i = m_i a_i$$

Also,

$$a_i = \frac{d^2 r_i}{dt^2}$$

We know that the force can also be expressed as the gradient of the potential function (5). Combining (5,6 and 7) we have

$$-\frac{dU(r_{ij})}{dr_{ij}} = m_i \frac{d^2 r_i}{dt^2}$$

Newton equation of motion then relates the derivative of the potential energy to change in position as a function of times. Due to the complicated nature of the potential function, there is no analytical solution to the equation of motion of the particles; they must be solved numerically.

The numerical algorithms developed for integrating the equation of motion include;

1. Verlet Algorithm
2. Verlet leap-frog Algorithm
3. Velocity Verlet Algorithm
4. Beeman's Algorithm

In choosing which Algorithm to use, one should consider the following criteria;

1. The algorithm should conserve energy
2. It should be computationally efficient
3. It should permit a long time-step for integration

Based on these criteria, the integration of the equation of motion in this work was done by using Leap-frog algorithm. The algorithm is simple but fast, It requires about a little memory and thus useful when we simulate but very large systems. In this algorithm, the velocities are first calculated at time = $\frac{1}{2} \Delta t$; these are used to calculate the positions, r , at time $t + \Delta t$, in this way, the velocities leap over the positions. The advantage of this algorithm is that the velocities are explicitly calculated, however, the disadvantages are that they are not calculated at the same time as the positions.

$$r(t + \Delta t) = r(t) + v(t + \frac{1}{2}\Delta t) \Delta t + O(\Delta t)^2$$

$$v(t + \frac{1}{2} \Delta t) = v(t - \frac{1}{2}\Delta t) + a(t) \Delta t + O(\Delta t)^2$$

The two equations are the based form of leap frog algorithm, where Δt is time step and $O(\Delta t)^2$ is the error term. The acceleration a , is calculated by dividing the force by the mass. And the force is in turn a function of the position,

That is,

$$a(t) = \frac{F}{m}$$

Also,

$$a(t) = -\frac{1}{M} \frac{dV(r)}{dr}$$

This algorithm requires that the force on all particles be computed rather frequently. The velocities at time t can be approximated by the relationship:

$$v(t) = v(t - \frac{1}{2} \Delta t) + a(t) \Delta t + O(\Delta t)^2$$

This expression is only accurate to order $(\Delta t)^2$

Calculation of samples

Samples are properties of interest of a *many* body system; these are quantities that can be compared with real experiments. Some properties of interest are the static and dynamical properties are the transport coefficients and the time correlation functions. The average values of properties are determined from the positions, velocities and accelerations of the particles obtained from the integration of the equations of motion.

The $g(r)$ measures how atoms organize themselves around one another. It is proportional to the probability of finding two atoms separated by distance r . The $g(r)$ can be evaluated from simulation data using:

$$g(r) = \frac{N(r, r)}{1/2 N_p V(r, r)}$$

$N(r, r)$ is the number of atoms found in a spherical shell of radius r and thickness Δr with the shell centered on another atom. $V(r, r)$ is the volume of the spherical shell. N is the total number of atoms. The internal energy is the average of the pair potential and it is given as

$$U = \int_0^L \rho \int_0^L f(r) dr$$

To calculate the pressure; we use:

$$P = \rho \int_0^L \frac{2}{r} \frac{du(r)}{dr} dr$$

When water surface is strikes with the blade of a paddle, the waters initial response to the sudden shock is a resistance to deformation much like that of a solid, resistance characterized by two elastic constants: the bulk modulus (the inverse isothermal compressibility) and the shear modulus (coefficient of rigidity). It is because of waters elastic resistance to a suddenly applied force that, if thrown hard and at low angle, a stone will skip across a lakes surface. For the Lennard-Jones substance, the shear modulus G is related to thermodynamics.

$$G = \frac{3P - \rho U}{2\rho K}$$

Where P and U are the pressure and the configurationally internal energy respectively.

The bulk modulus B is given

$$B = -\rho \left(\frac{\partial P}{\partial \rho} \right)_T$$

The work done by diffusing particles to shove other neighboring particles is given as

$$W = GV$$

Where V is the volume of the simulation box.

The shear force acting on the liquid generated a shear wave with a shear velocity given as

3.5 Computational Details

All simulations were performed in a cubic box of volume v with periodic boundary condition all three dimensions containing $N=500$ atoms of Nitrogen fluid modelled by the LJ potential. The equations of motion for the system were integrated using the Verlet leap-frog algorithm with a reduced time step of 0.004. Initial position and Lime were set to zero. The transport coefficients are calculated by averaging the appropriate auto-correlation functions. Thermo dynamical properties were also calculated. The length of the production phase depended on density and temperature of the state point. The total simulation time was 33,750 time steps. A total of 5 states were examined with temperature ranging from 20K-8 1K for the system. The density ranges from 1.039g/cm³ -0789g/cm³. mass, in of an atom is set to unity for convenience. Interactions beyond distance $r_c = L/2$ are set to zero. In this case, L is the length of the simulation box and r_c is the cut-off radius. Reduced temperature and density used are given as; $T^* = K_B T / \epsilon$ and $\rho^* = \rho \sigma^3$ respectively.

4.0 RESULTS AND DISCUSSIONS

4.1 Results

4.1.1 Thermodynamic state points of Nitrogen

T (K)	T*	$c(\text{g/cm}^3)$	c^*
20	0.197	1.030	1.065
63.13	0.622	0.870	0.899
66	0.650	0.857	0.886
77	0.758	0.808	0.835
81	0.797	0.789	0.815

4.1.2 Thermodynamic properties of Nitrogen

T	c	P	U_j
0.197	1.065	2.851	-7.621
0.622	0.899	0.783	-6.296
0.650	0.886	0.721	-6.190
0.758	0.835	0.441	-5.790
0.797	0.815	0.219	-5.657

4.1.3 Elastic properties of Nitrogen

T(K)	$c(\text{g/cm}^3)$	$G_{\text{md}}(\text{GP}_a)$	$G_{\text{exp}}(\text{GP}_a)$	$B_{\text{md}}(\text{GP}_a)$	$G_{\text{exp}}(\text{GP}_a)$
20	1.030	1.37	1.18	2.44	2.16
63.15	0.870	0.82	-	1.39	-
66	0.857	0.79	-	1.33	-
77	0.808	0.67	-	1.11	-
81	0.789	0.62	-	1.01	-

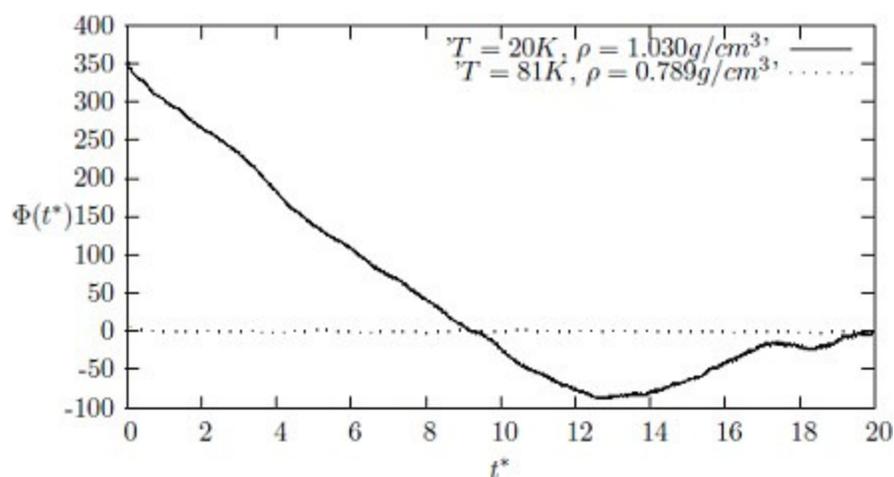


Figure 1. Stress autocorrelation function of Nitrogen at solid and liquid states

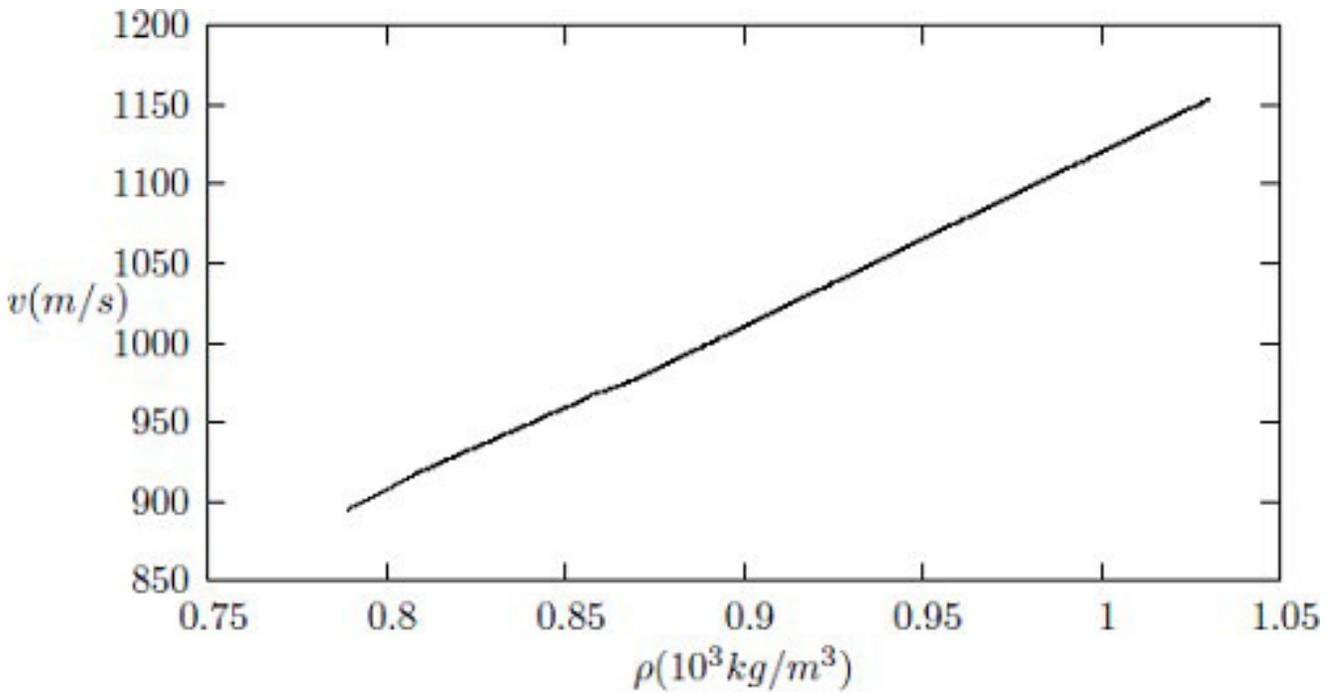


Figure2. *Speeds of shear waves in Nitrogen at the investigated densities*

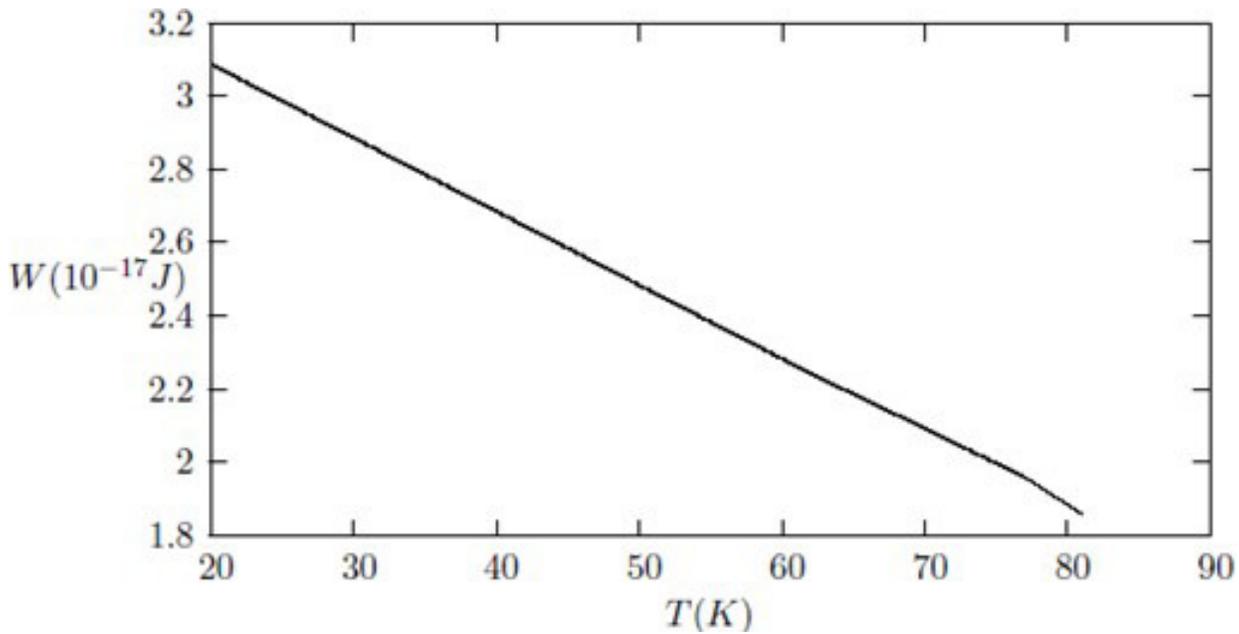


Figure3. *Work done by a diffusing particle of Nitrogen*

4.2 Discussion

Table 4.1.1 shows the thermodynamic state points at which the elastic and kinetic properties are calculated for nitrogen, it shows that as the temperature increases for nitrogen the density decreases. Table 4.1.2 shows the thermodynamic properties of nitrogen it indicates that as the density decreases with increase in temperature the internal energy increases and the pressure also decreases.

Table 4.1.3 shows the elastic properties of nitrogen from this table the shear modulus decreases and bulk modulus decreases, at $T=20\text{k}$ the shear and bulk compared well with experiments. Figure 1 present the graph plotted shows the stress autocorrelation function of nitrogen at solid and liquid states showing that (t^*) decreases as temperature increases. Figure 2 shows the graph plotted for the work done by a diffusing particle of nitrogen. The work done to shove aside neighboring particles by diffusing particles of nitrogen decreases as temperature increases. Figure 3 present the graph plotted shows the speed of shear waves in nitrogen at the investigated densities; As density increases the speed of the shear waves increases.

4.3 Computer Programs Used

4.3.1 Shear Modulus

PROGRAM SM

!

!This Program Calculates Shear Modulus

!

IMPLICIT NONE

REAL:: P,d,U,T, G=0.0

INTEGER:: K=1

PRINT* , Type in the values of P,d,U and T

PRINT* , Separate by spaces or commons

READ* P,d,U,T

$G = 3 * P - (24.0/5.0) * d * U - 2 * K * d * T$

PRINT* , shear modulus is, G

END PROGRAM

4.3.2 Bulk Modulus

PROGRAM BM

!

!This Program Calculates Bulk Modulus

!

IMPLICIT NONE

REAL:: P,d,T,G

PRINT* , Type in the values of P,d,T and G

PRINT* , Separate by spaces or commons

READ* P,d,T,G

$B = (5.0/3.0) * G + 2 * (P-d*K*T)$

PRINT* , Bulk modulus is, B

END PROGRAM

4.3.3 Work Done

W=GV

PROGRAM SM

!

!This Program Calculates Word Done

!

IMPLICIT NONE

REAL:: G,L, W=0.0

PRINT* , Type in the values of G and V

PRINT* , Separate by spaces or commons

READ* G,L

$W = G * (L ** 3.0)$

PRINT* , Work Done is, W

END PROGRAM Wd

4.3.3 Shear Waves Speed

PROGRAM SW

!

!This Program Calculates Shear Waves Speed,

!

IMPLICIT NONE

REAL:: G,d, U=0.0

PRINT* , Type in the values of G and d

PRINT* , Separate by spaces or commons

READ* G,d

W=(G/d)** 0.5

PRINT* , shear wave speed is, u

END PROGRAM SW

5. CONCLUSION AND SUGGESTION FOR FUTURE STUDIES

Using the method of molecular dynamic simulation, we have elastic and properties of liquid nitrogen at temperature range of 20K to 81K and density range of 0.789g/cm³ to 1.030g/cm³ using the Lennard-Jones potential: The calculated properties include the shear modulus and bulk modulus, shear waves speed, pressure, internal energy and work-done by diffusing particles of nitrogen. For comparison purpose, the shear modulus and bulk modulus of solid nitrogen were calculated at temperature 20K and there is a good agreement between calculated values and the experimental values. The study can be extended to complex liquids in the future.

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