Structure and Shear Modulus of the Neutron Star Crust

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Abstract. A thorough understanding of the neutron star crust is necessary to describe some observations of transient events such as quasi-periodic oscillations after magnetar giant flares and cooling following outbursts in low-mass X-ray binaries. I perform molecular dynamics simulations to model the crystalline structure of the crust and also compute shear modulus and liquid-solid phase diagrams.

1. Introduction

The structure of the neutron star (NS) crust can have important effects on observations of transient events such as quasiperiodic oscillations after magnetar giant flares[1] and cooling following an accretion-powered outburst in low-mass X-ray binaries[2]. The first question that needs to be asked when studying the crust is whether the solid crust is crystalline or amorphous. This difference can greatly affect transport properties. Ichimaru et al.[3] suggested that below the Wigner transition temperature, the OCP fluid may form an amorphous glassy state that could be long lived and thus should be taken into account when modeling NSs. Once the state of the NS crust is known, transport coefficients can be computed and these can be compared to observations.

In this paper, I will describe my molecular dynamics (MD) method in Section 2, determine whether the crust is crystalline or amorphous in Section 3, describe the shear modulus in Section 4, and conclude in Section 5.

2. Molecular Dynamics Formalism

In this section, I describe my MD formalism. For this work, I consider both a one component plasma (OCP) and mixture of two or three species. The ions interact via screened Yukawa interactions

\[ v_{ij}(r) = \frac{Z_i Z_j e^2}{r} e^{-r/\lambda}, \]

where \( Z_i \) and \( Z_j \) are the respective charges of the two ions being considered, \( r \) is the separation between the ions, and \( \lambda \) is the Fermi screening length, which for cold relativistic ions is

\[ \lambda^{-1} = 2k_F \sqrt{\frac{\alpha}{\pi}}. \]
Here, the electron Fermi momentum $k_F$ is
\[ k_F = (2\pi^2 n_e)^{1/3} \] and $\alpha$ is the fine structure constant. The electron density $n_e$ is equal to the ion charge density, $n_e = \langle Z \rangle n$, where $n$ is the ion density and $\langle Z \rangle$ is the average charge. My simulations are classical and I have neglected the electron mass (extreme relativistic limit).

One component plasma simulations can be characterized by the Coulomb parameter $\Gamma = Z^2 e^2 / aT$. I characterize my multicomponent system using an average Coulomb parameter,
\[ \Gamma = \langle Z^{5/3} \rangle \Gamma_e, \tag{3} \]
where $\Gamma_e = e^2 / a_e T$ with the electron sphere radius $a_e = (3/4\pi n_e)^{1/3}$.

Time can be measured in my system in units of one over the plasma frequency $\bar{\omega}_p$. For a one component plasma, the plasma frequency is
\[ \omega_p = \left[ 4\pi Z^2 e^2 n / M \right]^{1/2}, \tag{4} \]
where $M$ is the mass of the ion. For a mixture, I define an average plasma frequency and make an equation $\bar{\omega}_p = \left( 4\pi \langle Z \rangle^2 e^2 n / \langle M \rangle \right)^{1/2}$. Other choices for the average plasma frequency are expected to give very similar results.

3. Crust Structure

Here I describe the theoretical evidence that supports the NS crust being a crystalline solid, rather than amorphous. In order to see if the amorphous state is stable in the NS crust, I consider amorphous initial conditions. I start with a liquid configuration of $N = 8192$ ions that is equilibrated at $\Gamma = 175$. I then quench the system instantaneously to a large $\Gamma$ value by rescaling the velocities, and then evolve the system at (approximately) constant temperature until the system largely crystallizes. Table 1 lists the time needed to crystallize for different $\Gamma$ values. This time increases with increasing $\Gamma$. However, this time only increases approximately linearly with $\Gamma$ for $\Gamma < 1500$. This suggests that diffusion is relatively fast in the amorphous system, and that the amorphous to crystal transition does not involved a large energy barrier.

I find that the system is able to crystallize, even at $\Gamma = 1500$, where the temperature is 8.6 times lower than the melting temperature. However a final run that was quenched to $\Gamma = 1750$ was not observed to crystallize before a time $25,000,000 / \omega_p$. I refer to these quenched systems as amorphous, however it may be more appropriate to call them polycrystalline because they are observed to have many small crystal domains of different orientation. These polycrystalline states are observed to undergo rapid transitions to single crystals except at the largest $\Gamma$.

To quantify the crystalline order in these simulations, I consider a metric based on bond angles[4]. Ion $i$ is said to be bonded to ion $j$ if it is within a distance $b = 2.44a$ that corresponds to a minimum in the radial distribution function $g(r)$. This distance is chosen to include the eight nearest neighbors in a perfect body centered cubic (bcc) lattice. Let $\theta_{ij}$ and $\phi_{ij}$ be the polar and azimuthal angles of radius from ion $i$ to ion $j$. I calculate the spherical harmonic,
\[ Q_{lm} (\hat{r}_{ij}) = Y_{lm} (\theta_{ij}, \phi_{ij}), \tag{5} \]
and average over all $\approx 14N$ bonds for a given configuration,
\[ \bar{Q}_{lm} = \langle Q_{lm} (\hat{r}_{ij}) \rangle. \tag{6} \]
This quantity depends on the orientation of a crystal lattice with respect to the simulation volume. Therefore, I calculate the rotationally invariant quantity $Q_l[4],
\[ Q_l = \left[ \frac{4\pi}{2l+1} \sum_{m=-l}^{l} |Q_{lm}|^2 \right]^{1/2}. \tag{7} \]
Table 1. Approximate time $t_0$ for amorphous systems to crystallize, after the systems have been instantaneously quenched from $\Gamma = 175$ to different $\Gamma$ values. $N$ is the number of ions in the system.

| $N$   | $\Gamma$ | $t_0\omega_p$ |
|-------|----------|---------------|
| 8192  | 500      | 24,000        |
| 8192  | 600      | 47,000        |
| 8192  | 700      | 142,000       |
| 8192  | 1000     | 240,000       |
| 8192  | 1500     | 390,000       |
| 8192  | 1750     | >25,000,000   |
| 27648 | 500      | 400,000       |
| 27648 | 1000     | >6,000,000    |

This provides a measure of the crystalline order of a configuration. In general, $Q_l$ is small for a liquid or amorphous configuration and $Q_l$ is large for a perfect crystal. My calculations of $Q_l$, for a range of even $l$, show that $Q_6$ is most sensitive to crystalline order. I find that $Q_6 = 0.51069$ for a perfect, i.e. $T = 0$, bcc lattice, and $Q_6 = 0.57452$ for a perfect face centered cubic lattice. Note that $Q_l$ is small for odd $l$. In Figure 1 I show $Q_6$ versus simulation time $t_0$. However, the amount of time necessary for $Q_6$ to grow can increase strongly with increasing system size $N$ or $\Gamma$. A plateau near $Q_6 \approx 0.17$ is see for all four systems in Figure 1, which suggests a possible metastable intermediate state. The simulations with $N = 27648$ at $\Gamma = 500$ and $N = 8192$ at $\Gamma = 1500$ show a rapid rise in $Q_6$, near $t_0 = 4 \times 10^5/\omega_p$, during transitions to single crystals. For $N = 27648$ at $\Gamma = 1000$ and $N = 8192$ at $\Gamma = 1750$, $Q_6$ is increasing with time. These systems have not yet evolved into single crystals, however the continued rise of $Q_6$ with time strongly suggests that these sytems will evolve into single crystals at later times and are unlikely to remain amorphous.

I conclude that an amorphous solid will not form even with large amounts of supercooling, where the temperature is rapidly quenched by up to a factor of 10 below the melting temperature. Instead, diffusion is fast enough so that the system will form a regular crystal. My results strongly suggest that Coulomb solids in the interior of cold white dwarf stars and the crust of NSs will be crystalline and not amorphous. This is consistent with observations of rapid crust cooling of neutron stars following extended periods of accretion[2]. This rapid cooling implies a high crust thermal conductivity, that agrees with a the conductivity of a regular crystal, and is larger than that expected for an amorphous solid.

4. Shear Modulus

I now describe my methodology and results for the shear modulus in the NS crust. To calculate shear moduli, I follow the procedure of Ogata et al.[5]. The change in free energy with deformation $\delta F$ can be expressed in terms of elastic constants $c_{11}$, $c_{12}$, and $c_{44}$.

$$\delta F = \frac{1}{2} (c_{11} - c_{12}) u_{ii}^2 + c_{44} u_{ik} u_{ki} \quad (i \neq k), \quad (8)$$

and $u_{ik}$ describes the strain.

Under a deformation, the coordinates $r_k$ of an ion get mapped to $r_i'$,

$$r_i' = \sum_{k=1}^{3} (\delta_{ik} + u_{ik}) r_k. \quad (9)$$
I consider six deformations $D_i \ (i = 1 \ldots 6)$ that conserve the volume to order $\epsilon^2$.

\begin{align}
D_1 : \quad & u_{xx} = \epsilon + \frac{3}{4} \epsilon^2, \quad u_{yy} = u_{zz} = -\frac{\epsilon}{2} \\
D_2 : \quad & u_{yy} = \epsilon + \frac{3}{4} \epsilon^2, \quad u_{xx} = u_{zz} = -\frac{\epsilon}{2} \\
D_3 : \quad & u_{zz} = \epsilon + \frac{3}{4} \epsilon^2, \quad u_{xx} = u_{yy} = -\frac{\epsilon}{2} \\
D_4 : \quad & u_{xy} = u_{yx} = \frac{\epsilon}{2}, \quad u_{zz} = \frac{\epsilon^2}{4} \\
D_5 : \quad & u_{yz} = u_{zy} = \frac{\epsilon}{2}, \quad u_{xx} = \frac{\epsilon^2}{4} \\
D_6 : \quad & u_{zx} = u_{xz} = \frac{\epsilon}{2}, \quad u_{yy} = \frac{\epsilon^2}{4}
\end{align}

For each deformation $D_m$, I calculate a corresponding expectation value $f_m \ (m = 1 \ldots 6)$,

\[
f_m = \frac{1}{V} \left\{ \left\langle \left( \frac{d^2 V_{tot}}{d\epsilon^2} \right) \right\rangle - \frac{1}{T} \left[ \left\langle \left( \frac{dV_{tot}}{d\epsilon} \right)^2 \right\rangle - \left\langle \frac{dV_{tot}}{d\epsilon} \right\rangle^2 \right] \right\},
\]

where $V$ is the system volume and $V_{tot}$ is the total potential under deformation $D_m$. At zero temperature, this reduces to $f_m = (d^2 V_{tot}/d\epsilon^2)/V$.

For a bcc crystal, one has $f_1 = f_2 = f_3 = 3b_{11} = 3(c_{11} - c_{12})$ and $f_4 = f_5 = f_6 = c_{44}$. Here, $c_{11}$, $c_{12}$, and $c_{44}$ are elastic constants. In practice I calculate all six $f_m$ independently and
average to determine $b_{11}$ and $c_{44}$. The angle averaged shear modulus is\[5, \]

$$
\mu_{\text{eff}} = \frac{2b_{11} + 3c_{44}}{5}.
$$

(17)

If the NS crust involves many crystal domains of random orientation, then $\mu_{\text{eff}}$ is the appropriate elastic constant to determine the speed of shear waves.

For simplicity, I work at a density $n = 7.18 \times 10^{-5} \text{ fm}^{-3}$ and $Z = 29.4$. My results can be scaled to other densities at a given value of $\Gamma$. My results can also be approximately scaled to other values of $Z$, at fixed $\Gamma$. This is because, although the ratio of $\lambda/a$ changes with $Z$, this change in screening has only a small effect on the shear modulus. I evolve the system with the velocity Verlet algorithm\[6\] using a time step $\delta t = 25 \text{ fm}/c$. Starting from $T = 0$ and a perfect fcc lattice, I increase the temperature to $T = 0.1 \text{ MeV}$ and evolve the system for typically 100000 MD steps ($2.5 \times 10^6 \text{ fm}/c$) to reach thermal equilibrium. Next, I evolve for a further 250000 MD steps ($6.25 \times 10^6 \text{ fm}/c$) storing configurations for later calculations of elastic constants. The temperature is then raised by $0.1 \text{ MeV}$ and the process is repeated. I keep the system at a fixed temperature (approximately) by periodically rescaling the velocities. These MD simulations are done in an undistorted cubic box using periodic boundary conditions.

I calculate $f_m$ by averaging over 1000 configurations, each separated by 250 MD steps. To minimize finite size effects, I calculate $V_{\text{tot}}$ by summing over all 27 nearest periodic images. Thus ion $i$ is assumed to interact not only with ion $j$ at its original position, but also with 26 more images of $j$ where the $x$, $y$, and $z$ coordinates are independently shifted by $0$, $+l$, or $-l$, with $l$ being the box size. The derivatives in Equation 16 are approximated using a five point numerical formula. I note that the MD trajectories have been calculated using periodic distances (involving only the single nearest periodic image of a given ion) to save time, while the derivatives have been calculated by summing over 27 images to minimize finite size effects.

Table 2 presents results for simulations using $N = 3456$ ions. Statistical errors only are indicated in parentheses. I caution that $b_{11}$ may have significant errors from finite size and other systematic effects. I fit the values of $\mu_{\text{eff}}$ in Table 2 with a simple analytic formula that is valid for all $\Gamma \geq 175$,

$$
\mu_{\text{eff}} \approx \left( 0.1106 - \frac{28.7}{\Gamma^{1.3}} \right) \left( n \frac{Z^2 e^2}{a} \right)
$$

(18)

This fit has an error $\leq 2\%$.

### Table 2. Shear moduli for MD simulations with $N = 3456$ ions in units of $nZ^2e^2/a$.

| $\Gamma$ | $b_{11}$ | $c_{44}$ | $\mu_{\text{eff}}$ |
|----------|---------|---------|------------------|
| $\infty$ | 0.0220  | 0.1699  | 0.1107           |
| 834      | 0.0209(2)| 0.1617(3)| 0.1054(2)       |
| 417      | 0.0194(2)| 0.1517(3)| 0.0988(2)       |
| 278      | 0.0202(4)| 0.1410(5)| 0.0927(3)       |
| 200      | 0.0154(5)| 0.1253(10)| 0.0813(6)      |
| 175      | 0.0158(8)| 0.1152(10)| 0.0755(6)       |

To study finite size effects, I have performed additional simulations with larger and smaller systems of sizes $N = 9826$ and $N = 1024$, respectively. Since the $\mu_{\text{eff}}$ is about 1% smaller for $N = 9826$ compared to $N = 3456$, I estimate finite size effects to be of order 1%. Figure 2 plots these results for $\mu_{\text{eff}}$ and also shows the Monte Carlo results of Ogata et al.\[5\]. These results are about 10% larger than my results at large $\Gamma$ and have much larger statistical errors.

Ogata et al. neglect electron screening $\lambda \to \infty$. At zero temperature, I have performed calculations for larger values of $\lambda$ and extrapolated to $\lambda \to \infty$. My extrapolated results are
Figure 2. Angle averaged shear modulus $\mu_{eff}$ versus Coulomb parameter $\Gamma$ for MD simulations involving $N = 1024$, 3456, and 9826 ions. Also shown are Monte Carlo results from Ogata et al.[5] that omit electron screening.

consistent with Ogata et al. Therefore, I conclude that electron screening reduces $\mu_{eff}$ be about 10%. The speed of shear waves is proportional to the square root of $\mu_{eff}$, so electron screening reduces shear speed by about 5%. This will slightly lower the frequency of torsional oscillations of neutron star crusts.

5. Conclusion
I have shown that the NS crust is most likely crystalline. The fact that amorphous systems are unstable to spontaneous crystallization suggests that macroscopic sections of the NS crust should be a regular crystal. Observational results also suggest that the crust is crystalline since the low thermal conductivity of an amorphous solid cannot explain observations.

Since the crust is most likely crystalline, the shear modulus can be computed including the effect of electron screening that was neglected in previous calculations. Including electron screening reduces the shear modulus by about 10% which implies a corresponding reduction in shear speed of 5%. This difference should be observable with high quality data of quasi-periodic oscillations after magnetar giant flares.

References
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