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Molecular Dynamics Simulations of Accreting Neutron Star Crust

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Material accreting on a neutron star can undergo rapid proton capture nucleosynthesis to produce a variety of nuclei up to mass numbers around 100. This complex rp ash then undergoes electron capture as it is buried to higher densities. We perform molecular dynamics simulations to determine how this material freezes to form new neutron star crust. In addition, from our simulations we calculate many properties of crust made of this complex rp ash composition including thermal conductivity, viscosity, and shear modulus. We also calculate the strong screening enhancement of nuclear reaction rates. Finally, we are determining the breaking strain (strength) of the crust. This is important for the height of mountains that radiate gravitational waves and may be important for giant flares (extremely energetic gamma / X-ray bursts) from very strongly magnetized neutron stars called Magnetars. These flares may originate in a star quake when magnetic stress breaks the crust.

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Neutron stars in binary systems can accrete material from their companions. As gas falls onto the neutron star, it can undergo rapid proton capture nucleosynthesis where seed nuclei rapidly capture protons to make a series of proton rich nuclei up to mass numbers A around 100. For example H. Schatz et al. [1] have calculated the composition remaining when rapid proton capture is finished. Next Gupta et al. have calculated how electron capture changes the composition of the rp ash as further accretion buries it to higher densities where it is subject to a large electron density [2].

Next the material is expected to freeze when it reaches densities of order 10^{10} g/cm^3, At these densities Coulomb interactions between ions dominate over thermal fluctuations and a body centered cubic crystal is expected to form. This process allows accretion to make new neutron star crust. What happens to the complex rp ash composition when it freezes? In previous work, large scale molecular dynamics simulations find that chemical separation takes place as the material freezes [3]. The liquid ocean is enriched in low charge Z elements while the solid crust is enriched in high Z elements.

Molecular dynamics simulations are also used to calculate many properties of the rp ash crust. The thermal conductivity is important for how the crust cools. Recently crust cooling was observed for two neutron stars after extended outbursts [4]. Accretion over several years heated the crust out of equilibrium. Then when the accretion stopped, the crust cooling time was measured. This cooling time is very sensitive to the thermal conductivity and comparisons of the observations with simulations strongly suggest that the crust has a high thermal conductivity [5]. This would be expected if the crust forms a regular lattice with small impurity concentrations. An amorphous crust has a low thermal conductivity and is strong disfavored by the observations. The thermal conductivity is dominated by heat carried by electrons and this is limited by electron-ion scattering. In ref. [6] we calculate the static structure factor $S(q)$ for electron-ion scattering using molecular dynamics simulations including many impurities. From $S(q)$ we determine the thermal conductivity.

Nuclear fusion reactions in the crust can provide heat and help determine the temperature profile. Pycnonuclear reactions are driven by quantum zero point motions at high densities while thermonuclear reactions are driven by thermal fluctuations. The rates of these reactions are greatly enhanced by the screening of the Coulomb barrier provided by other ions [7]. In ref. [8] we calculate this screening and estimate that ^{24}O + ^{24}O fusion will occur at densities near 10^{11} g/cm^3. This assumes a simple barrier penetration model for the astrophysical S factor. We note that fusion of very neutron rich light nuclei such as ^{24}O could be greatly enhanced by the dynamics of the neutron skin. This is a very interesting nuclear structure question that should be studied in the laboratory with radioactive beams.

Finally we discuss mechanical properties of the crust including its shear modulus and breaking strain. Magnetar giant flares are extraordinarily energetic gamma and X-ray bursts that are thought to involve large scale magnetic field reconnection in very strongly magnetized neutron stars. Quasiperiodic oscillations have recently been observed in giant flares. These may correspond to torsional oscillations of the neutron star crust. If true the spectrum of observed modes could yield detailed information on the crust. The frequencies of these modes depends on the shear modulus μ of the crust. Our new molecular dynamics simulations of the shear modulus [9] find that electron screening reduces μ by about 10% compared to earlier Monte Carlo calculations of Ogata et al. [10]. In addition rp ash impurities can reduce μ by up to 50%.

One model for giant flares has magnetic stress causing the crust to break and move. This allows the magnetic field to reconnect and radiate the flare [11]. This may require the crust to be very strong in order to control fields large enough to generate the great flare energy. Unfortunately, very little is known about the breaking strength of the crust and we are not aware of any previous breaking strain simulations. In addition the breaking strain is also important for gravitational wave radiation. Large bumps on a rotating neutron star (mountains) will radiate gravitational waves. This radiation could be detected in LIGO and may limit the rotational frequencies of accreting neutron stars [12]. The height of these mountains, and the gravitational waves they radiate, is limited by the crust breaking strain [13]. This determines when mountains collapse under their own weight. Note that LIGO has already set some limits on mountains [14] and has searched for gravitational waves during Magnetar giant flares [15].

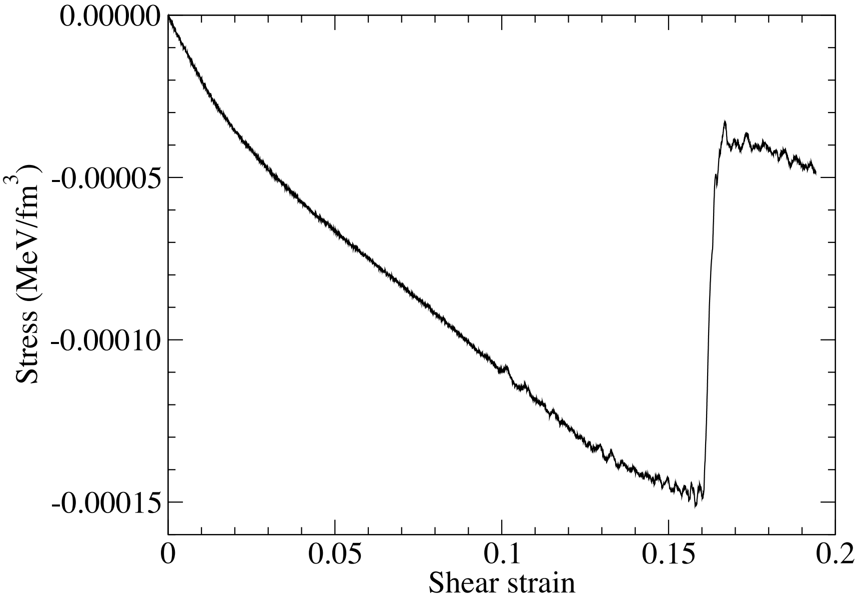

Figure 1: The stress (force per unit area) versus strain (fractional deformation) of a 3456 ion simulation.

We are starting to perform MD simulations of the breaking strain. The strain is the fractional deformation of the crystal. We strain a simulation volume by slowly deforming the boundaries from a cube into a parallelogram. We calculate the resulting force per unit area (Stress) that resists this deformation. In Fig. 1 we show the stress for a 3456 ion simulation at a density of 7.18×10^{-5} fm^{-3} and a temperature of $T = 0.1$ MeV. Each ion is assumed to have the same charge $Z = 29.4$ and the shear rate is 8×10^{-8} c/fm. Figure 2 shows the simulation just as the crust is breaking. The breaking strain depends on simulation size and shear rate. In future large scale MD simulations in collaboration with Kai Kadau, we will perform breaking strain simulations with much larger systems in order to estimate the large scale breaking strain of neutron star crust [16] and how this depends on impurities and defects.

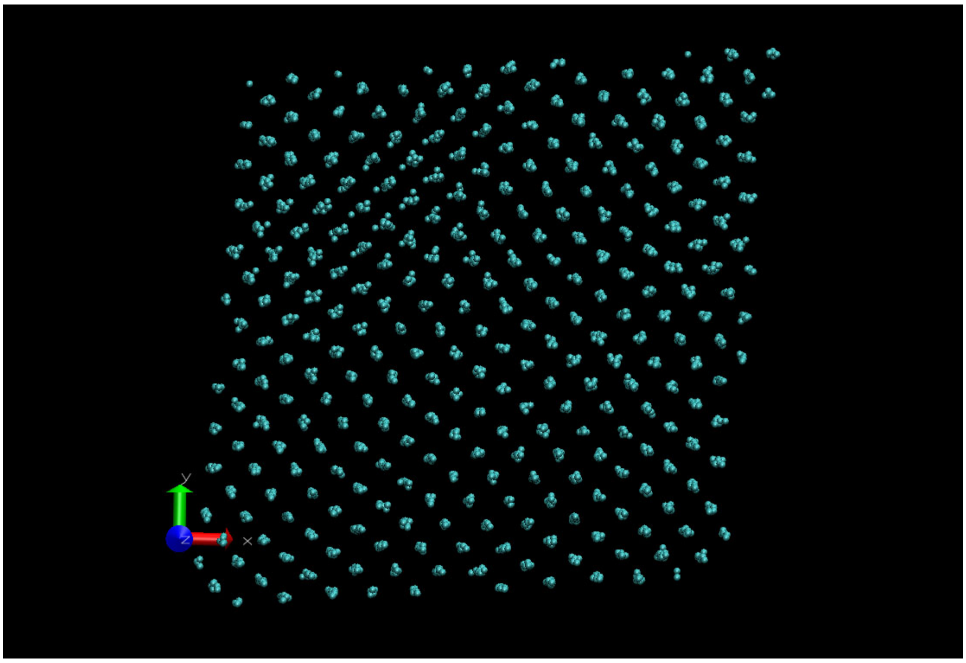

Figure 2: Configuration of 3456 ions at a shear near 0.16. The crystal is just starting to break in the upper left quadrant of the image as indicated by a some ions moving from their lattice sites.

In conclusion, we are performing molecular dynamics simulations to determine many properties of the crust of accreting and isolated neutron stars. The crust of accreting stars may have a complex composition with many impurities. Properties we are calculating include phase separation, thermal conductivity, shear viscosity, shear modulus, and breaking strain. These are important for X-ray and gravitational wave radiations.

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References

[1] H. Schatz et al., PRL **86** (2001) 3471.

[2] S. Gupta, E. F. Brown, H. Schatz, P. Moller, and K-L. Kratz, ApJ **662** (2007) 1188.

[3] C. J. Horowitz, D. K. Berry, and E. D. Brown, PRE **75** (2007) 066101.

[4] R. Wijnands et al., astro-ph/0405089. E. M. Cackett et al., astro-ph/0605490.

[5] R. E. Rutledge et al., astro-ph/0108125. P. S. Shternin, D. G. Yakovlev, P. Haensel, and A. Y. Potekhin, arxiv:0708.0086.

[6] C. J. Horowitz, O. L. Cabalero and D. K. Berry, arxiv:0804.4409.

[7] D. G. Yakovlev, L. R. Gasques, M. Beard, M. Wiescher, and A. V. Afanasjev, PRC **74** (2006) 035803.

[8] C. J. Horowitz, H. Dussan, and D. K. Berry, PRC **77**(2008) 045807.

[9] C. J. Horowitz and J. Hughto, to be published.

[10] S. Ogata and S. Ichimaru, PRA **42** (1990) 4867.

[11] C. Thompson, M. Lyutikov, and S. R. Kulkarni, ApJ. **574** (2002) 332.

[12] A. L. Watts, B. Krishnan, L. Bildsten, and B. F. Schutz, MNRAS **389** (2008) 839.

[13] G. Ushomirsky, C. Cutler, and L. Bildsten, MNRAS **319** (2000) 902.

[14] LIGO Scientific collaboration, arxiv:gr-qc/0702039.

[15] LIGO Scientific collaboration et al., arxiv:0808.2050.

[16] C. J. Horowitz and K. Kadau, to be published.