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Elastic properties of binary crystals in neutron stars and white dwarfs

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ABSTRACT

Elastic properties play an important role in neutron stars and white dwarfs. They are crucial for modelling stellar oscillations and different processes in magnetars and in degenerate stars, which enter compact binary systems. Using electrostatic energy of deformed lattices, we calculate elastic moduli of ordered binary body-centred cubic (sc2) and face-centred cubic lattices. We use two methods to determine the effective shear modulus $\mu_{\rm eff}$. We show that $\mu_{\rm eff}$ calculated as an average of the shear stiffness over all possible wavevectors (for polarization vectors perpendicular to the wave vector) agrees with the results obtained from the linear mixing rule. For the sc2 lattice, our calculations are also consistent with the results of numerical simulations of disordered binary body-centred cubic lattice.

Key words: dense matter – stars: neutron – white dwarfs.

1 INTRODUCTION

It is usually thought that outer crusts of neutron stars and cores of old white dwarfs consist of weakly polarized degenerate electrons and fully ionized atoms arranged into a crystal lattice (e.g. Shapiro & Teukolsky 1983; Haensel, Potekhin & Yakovlev 2007). This system could be described by the model of a Coulomb crystal of ions, where ions are treated as point particles while electrons form a uniform or weakly polarizable neutralizing background. Note that the inner crust of a neutron star contains also neutrons, which weakly affect electron–ion interaction; the Coulomb crystal model can be extended for this part of the crust too. The model of the Coulomb crystal allows one to study thermodynamic (e.g. Baiko, Potekhin & Yakovlev 2001), transport (e.g. Potekhin et al. 1999), and others properties of stellar matter (e.g. Chamel & Haensel 2008). In this paper, we focus on static elastic properties of Coulomb solids in the interiors of degenerate stars.

The study of elastic properties of the crust is a very important issue in physics of neutron stars, especially in physics of their oscillations. Strohmayer et al. (1991) demonstrated that toroidal, spheroidal and interfacial oscillation modes significantly depend on the effective shear modulus $\mu_{\rm eff}$. In turn, toroidal modes are used for the interpretation of global seismic oscillations of soft gamma repeaters (e.g. Duncan 1998) and quasi-periodic oscillations of magnetars (e.g. Strohmayer & Watts 2006; Gabler et al. 2018). According to some models, the magnetar activity is generated by shear motions near the neutron star surface and therefore depends on $\mu_{\rm eff}$ (Beloborodov & Levin 2014; Li, Levin & Beloborodov 2016). The problem of mountain formation on the neutron stars surface is directly related to the elastic properties. These mountains can be efficient sources of gravitational waves (e.g. Ushomirsky, Cutler & Bildsten 2000; Haskell, Jones & Andersson 2006; Johnson-McDaniel & Owen 2013; Haskell & Patruno 2017; Abbott et al. 2019). Hence, the effective shear modulus is required to interpret different sets of observational data. In this way it serves as an important microphysical parameter of neutron star envelopes.

Many previous publications considered lattices in neutron stars and white dwarfs as one-component. In addition it was often thought that the ions form the body-centred cubic (bcc) Coulomb lattice (e.g. Chamel & Fantina 2016). The elastic moduli of the bcc lattice were investigated in several works (Fuchs 1936; Wallace 1967; Robbins, Kremer & Grest 1988; Ogata & Ichimaru 1990; Strohmayer et al. 1991; Igarashi & Iyetomi 2003; Horowitz & Hughto 2008; Baiko 2011, 2015) both numerically and analytically. For instance, Ogata & Ichimaru (1990); Strohmayer et al. (1991) employed the Monte Carlo method and analysed free energy changes during lattice deformations. In this approach, elastic moduli of the static lattice are determined through a limit of free energy changes at $T = 0$.

However, investigations of multicomponent crystals are certainly important, particularly, for compact binaries (containing a neutron star or/and a white dwarf). These systems are interesting not only as the sources of gravitational waves but also as the objects for studying intensive accretion processes. Simulations show that neutron star crust in a compact binary can be very heterogeneous as far as its ion composition is concerned (e.g. Daligault & Gupta 2009; Horowitz & Berry 2009; Caplan et al. 2018).

Note that the cores of white dwarfs are composed of carbon–oxygen mixture with traces of other elements (e.g. Segretain et al. 1994). During the thermal evolution, such a mixture crystallizes with the formation of a multicomponent Coulomb crystal (e.g. Althaus et al. 2010).

Previously, elastic properties of multicomponent Coulomb compounds have been studied, as far as we know, only numerically for binary lattices in the disordered state (i.e. neglecting correlations in positions of different ions) by Igarashi & Iyetomi (2003).

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In the present paper, we calculate the elastic properties of one-component and binary ordered Coulomb lattices. We use the zero temperature limit and consider only static elastic properties. It is a good approximation for internal neutron star temperatures below 10^8 K (e.g. Gearheart et al. 2011). We examine two different approaches to calculate $\mu_{\rm eff}$ (see Kobyakov & Pethick 2015, for a review) and two types of crystal lattices. We discuss also the applicability of the linear mixing rule to determine the elastic moduli. The influence of the finite temperature to the multicomponent systems may be valuable for young neutron stars and could be studied via thermodynamic perturbation theory (Baiko 2011, 2015) or molecular dynamic simulations (Horowitz & Hughto 2008).

The present paper is organized as follows. Section 2 discusses electrostatic energies of a binary bcc lattice stretched along the edges of the basic lattice cube. These energies are used to calculate the elastic coefficients of the binary bcc lattice in Section 3 and the effective shear modulus in Section 4. The importance of screening corrections is discussed in Section 5. The elastic coefficients and the effective shear modulus of the binary face-centred cubic lattice are studied in Section 6. Astrophysical implications are outlined in Section 7.

2 ELECTROSTATIC ENERGY

Consider the simplest case of multicomponent Coulomb crystals – an ordered binary body-centred cubic (sc2) lattice. Following Kozhberov & Baiko (2012, 2015), we describe it as a simple cubic lattice with two ions in the elementary cell ($N_{\rm cell}=2$). So we use the main translation vectors for the sc2 lattice, $\mathbf{a}_1 = a_{\rm l}(1,\,0,\,0)$, $\mathbf{a}_2 = a_{\rm l}(0,\,1,\,0)$, and $\mathbf{a}_3 = a_{\rm l}(0,\,0,\,1)$ and the basis vectors $\boldsymbol{\chi}_1 = 0$, $\boldsymbol{\chi}_2 = 0.5a_{\rm l}(1,\,1,\,1)$, where $a_{\rm l}$ is the lattice constant. The basis vector $\boldsymbol{\chi}_1$ corresponds to the ion with the charge number Z_1 and the basis vector $\boldsymbol{\chi}_2$ corresponds to the ion with the charge number Z_2. The origin of a Cartesian coordinate system is chosen such that $Z_2 \geq Z_1$. The number density of ions with the charge number Z_1 is denoted as n_1, and the number density of other ions is n_2 (in the sc2 lattice $n_1 = n_2$).

According to Kozhberov & Baiko (2012, 2015), the electrostatic energy of the ordered multicomponent lattice can be written as

$$
\begin{aligned}
U_{\rm M} &= N\frac{Z_1^2e^2}{a}\xi\,,\\
\xi &= \frac{a}{2N_{\rm cell}}\sum_{lpp'}\frac{Z_pZ_{p'}}{Z_1^2}\left(1-\delta_{pp'}\delta_{\mathbf{R}_l0}\right)\frac{\operatorname{erfc}\left(AY_{lpp'}\right)}{Y_{lpp'}}\\
&\quad-\frac{Aa}{N_{\rm cell}\sqrt{\pi}}\sum_{p}\frac{Z_pZ_{p'}}{Z_1^2}-\frac{3}{8N_{\rm cell}^2A^2a^2}\sum_{pp'}\frac{Z_pZ_{p'}}{Z_1^2}\\
&\quad+\frac{3}{2N_{\rm cell}^2a^2}\sum_{mpp'}\frac{Z_pZ_{p'}}{Z_1^2}(1-\delta_{\mathbf{G}_m0})\\
&\quad\times\frac{1}{G_m^2}\exp\left[-\frac{G_m^2}{4A^2}+i\mathbf{G}_m(\boldsymbol{\chi}_p-\boldsymbol{\chi}_{p'})\right]\,,
\end{aligned}
\tag{1}
$$

where $\mathbf{Y}_{lpp'} = \mathbf{R}_l + \boldsymbol{\chi}_p - \boldsymbol{\chi}_{p'}$, $\mathbf{R}_l = l_1\mathbf{a}_1 + l_2\mathbf{a}_2 + l_3\mathbf{a}_3$ are the lattice vectors; l_1, l_2, andl_3 are arbitrary integers; $\mathbf{G}_m = m_1\mathbf{g}_1 + m_2\mathbf{g}_2 + m_3\mathbf{g}_3$ are the vectors of reciprocal lattice; $\mathbf{g}_i\mathbf{a}_j = 2\pi\delta_{ij}$; m_1, m_2, and m_3 are arbitrary integers; sums over p and p' go over all ions in the elementary cell (in the ordered crystal the charge number of an ion Z_p depends only on its place in the elementary cell); $\operatorname{erfc}(x)$ is the complementary error function; N is the total number of ions; $a\equiv(4\pi n/3)^{-1/3}$ is the ion sphere radius; n is the total number density of ions (for the sc2 lattice, $n = n_1 + n_2 = 2n_1$). A is an arbitrary parameter ($Aa\approx1$), which is chosen to optimize the convergence of summation in equation (1) and $U_{\rm M}$ is independent of A.

Table 1. Parameters of the approximation of the Madelung constant of the stretched sc2 lattice.

	$K_1(c_1,c_2)$		$K_2(c_1,c_2)$	
i	m_i	n_i	x_i	y_i
0	−0.061 6385		−0.372 2545	
1	−0.301 618	−0.385 7925	0.776 568	0.010 696
2	0.474 446	0.042 8725	−0.793 227	0.021 387
3	−0.202 857	0.092 4215	0.240 636	0.100 33
4	0.041 644	−0.045 568	−0.021 922	−0.044 87

The parameter ξ is the Madelung constant. For any binary crystal it depends only on $\alpha\equiv Z_2/Z_1$. For the sc2 lattice

$$
\begin{aligned}
\xi_{\rm sc2} &= \frac{1+\alpha^2}{2^{4/3}}\xi_1+\alpha\left(\xi_2-\frac{\xi_1}{2^{1/3}}\right)\\
&= -0.349\,2518\left(1+\alpha^2\right)-0.197\,4256\alpha\,,
\end{aligned}
\tag{2}
$$

where $\xi_1 = \xi_{\rm sc} = -0.880\,059\,442\,11$ is the Madelung constant of the simple cubic (sc) lattice and $\xi_2 = \xi_{\rm bcc} = -0.895\,929\,255\,68$ is the Madelung constant of the bcc lattice.

Equation (1) allows one to calculate the electrostatic energy of any periodic multicomponent lattice, in particular the sc2 lattice with arbitrary uniform deformation. In this section, we consider the sc2 lattice stretched along edges of the main lattice cube in such a way that the main translation vectors tend to be $\mathbf{a}_1 = a_{\rm l}(1,\,0,\,0)$, $\mathbf{a}_2 = a_{\rm l}(0,\,c_1,\,0)$, $\mathbf{a}_3 = a_{\rm l}(0,\,0,\,c_2)$, where the parameters c_1 and c_2 characterize the stretch value. In the common case the volume of the elementary cell changes during the stretching ($na_{\rm l}^3 = 2/(c_1c_2)$ at arbitrary c_1 and c_2). It is stay constant only at $c_2 = 1/c_1$.

The Madelung constant $\xi(c_1,\,c_2)$ of the stretched sc2 lattice depends on α, c_1, and c_2. For $1.0\leq c_1,\,c_2\leq1.6$ it can be approximated as

$$
\begin{aligned}
\xi(c_1,c_2) &= K_1(c_1,c_2)(1+\alpha^2)+K_2(c_1,c_2)\alpha,\\
K_1(c_1,c_2) &= \sum_{i=0}^{4}m_i\left(c_1^i+c_2^i\right)+n_1c_1c_2\\
&\quad+n_2c_1^2c_2^2+n_3\left(c_1^2c_2+c_1c_2^2\right)+n_4\left(c_1^3c_2+c_1c_2^3\right),\\
K_2(c_1,c_2) &= \sum_{i=0}^{4}x_i\left(c_1^i+c_2^i\right)+y_1c_1c_2\\
&\quad+y_2c_1^2c_2^2+y_3\left(c_1^2c_2+c_1c_2^2\right)+y_4\left(c_1^3c_2+c_1c_2^3\right).
\end{aligned}
\tag{3}
$$

The parameters of the approximation m_i and n_i are presented in Table 1. Errors of the approximation do not exceed 0.02 per cent.

At any fixed Z_1 and Z_2 the electrostatic energy of the stretched sc2 lattice reaches its minimum at $c_1 = 1$ and $c_2 = 1$, so that the bcc lattice does not change its shape when α changes. Note that in the binary hexagonal close packed lattice the distance between hexagonal layers decreases with increasing α (Kozhberov 2018).

3 ELASTIC COEFFICIENTS

In some cases it is convenient to rewrite the Madelung constant as

$$
\xi' \equiv \xi\frac{2a_{\rm l}}{a}\,.
\tag{4}
$$

For the sc2 lattice, $na_1^3 = 2$; hence, $a_1^3 = 8\pi a^3/3$ and

$$\xi'_{\rm sc2} = 4(\pi/3)^{1/3}\xi_{\rm sc2}\,. \tag{5}$$

For the stretched sc2 lattice,

$$\xi'(c_1, c_2) = 4\left(\frac{\pi}{3c_1c_2}\right)^{1/3}\xi(c_1, c_2)\,. \tag{6}$$

If lattice deformations are small, we can expand $\xi'(c_1, c_2)$ in powers of $c_1 - 1$ and $c_2 - 1$,

$$\begin{aligned}\xi'(c_1, c_2) \approx{}& \xi'_{\rm sc2} - \tilde{p}'_{\rm sc2}\left[(c_1 - 1) + (c_2 - 1)\right]\\ &+ 0.25\tilde{s}^{\rm xxxx}_{\rm sc2}\left[(c_1 - 1)^2 + (c_2 - 1)^2\right]\\ &+ 0.5\tilde{s}^{\rm xxyy}_{\rm sc2}(c_1 - 1)(c_2 - 1)\,,\end{aligned} \tag{7}$$

where $\tilde{p}'_{\rm sc2} = \xi'_{\rm sc2}/3$ is the electrostatic pressure (this equality is valid for any lattice with the isotropic pressure). The parameters $\tilde{s}^{\rm xxxx}_{\rm sc2}$ and $\tilde{s}^{\rm xxyy}_{\rm sc2}$ are the static lattice elastic coefficients

$$\tilde{s}^{\rm xxxx}_{\rm sc2} = 0.32969383(1 + \alpha^2) - 2.144195558\alpha\,, \tag{8}$$

$$\tilde{s}^{\rm xxyy}_{\rm sc2} = -0.637729828(1 + \alpha^2) + 0.804785789\alpha\,. \tag{9}$$

At $\alpha = 1$ the sc2 lattice tends to the bcc lattice. Hence $\tilde{s}^{\rm xxxx}_{\rm bcc} = -1.484\,807\,92$ and $\tilde{s}^{\rm xxyy}_{\rm bcc} = -0.470\,673\,87$. For the bcc lattice these elastic coefficients were obtained earlier (Fuchs 1936; Ogata & Ichimaru 1990; Baiko 2011). Baiko (2011) denoted them as $S^{\rm st}_{1111}$ and $S^{\rm st}_{1122}$, respectively, and our results fully reproduce them. Note that $\tilde{s}^{\rm xxxx} + 2\tilde{s}^{\rm xxyy} = 2\tilde{p}'$ for any cubic Coulomb lattice (Chugunov 2019).

The ideal cubic crystal lattice has three independent elastic moduli. Two of them are $\tilde{s}^{xxxx}$ and $\tilde{s}^{xxyy}$. The third static lattice elastic modulus can be found from the analysis of the electrostatic energy of the sc2 lattice with a shift. In the elementary cell of this lattice the top layer is horizontally shifted with respect to the bottom layer (cube of the elementary cell turns to a square based prism). The main translation vectors of the sc2 lattice with a shift can be defined as $\mathbf{a}_1 = a_1(1, 0, 0)$, $\mathbf{a}_2 = a_1(0, 1, 0)$, and $\mathbf{a}_3 = a_1(c_x, c_y, 1)$. In this case the volume of the elementary cell does not change during deformation and $na_1^3 = 2$.

The Madelung constant of the sc2 lattice with a shift $\xi'(c_x, c_y)$ depends on α and on parameters of deformation c_x and c_y. At small c_x and c_y the quantity $\xi'(c_x, c_y)$ can be written as

$$\xi'(c_x, c_y) \approx \xi'_{\rm sc2} + 0.25\tilde{s}^{\rm xyxy}_{\rm sc2}\left(c_x^2 + c_y^2\right)\,, \tag{10}$$

$$\tilde{s}^{\rm xyxy}_{\rm sc2} = -0.164846915(1 + \alpha^2) + 1.072097779\alpha. \tag{11}$$

For the bcc lattice, we have $\tilde{s}^{\rm xyxy}_{\rm bcc} = 0.742\,403\,95$, which agrees with the result of Baiko (2011) where this coefficient is denoted as $S^{\rm st}_{1212}$. One can see that, numerically, $\tilde{s}^{\rm xyxy}_{\rm sc2} = -\tilde{s}^{\rm xxxx}_{\rm sc2}/2$.

In equations (8, 9, and 11) the static lattice elastic coefficients and the pressure are presented in dimensionless units. In physical units we can write that for the sc2 lattice

$$\begin{aligned}s^{xyxy}_{\rm sc2} &= n\frac{Z_1^2e^2}{2a_1}\tilde{s}^{xyxy}\\ &= n\frac{Z_1^2e^2}{2a_1}\left(-0.164846915(1 + \alpha^2) + 1.072097779\alpha\right).\end{aligned} \tag{12}$$

In some papers (e.g. Ogata & Ichimaru 1990; Baiko 2015) the elastic coefficients are measured in units of a instead of $2a_1$. Then, for instance,

$$c_{44} \equiv s^{\rm xyxy}\frac{a}{2a_1}\,, \quad c_{44,\rm bcc} = 0.18276965n\frac{Z_1^2e^2}{a}\,. \tag{13}$$

Table 2. Values of c_{44} in units of $nZ_1^2e^2/a$ for the binary bcc lattice.

α	4/3	2	3
$c_{44,\rm sc2}$	0.239 184	0.324 956	0.385 977
$c^{\rm dis}_{44,\rm sc2}$	0.241	0.292	0.549
$c^{\rm lm}_{44,\rm sc2}$	0.251 59	0.436 72	0.833 63

Previously, elastic coefficients of multicomponent lattices have been studied only via molecular dynamic simulations by Igarashi & Iyetomi (2003), and only the disordered binary bcc lattice has been considered (in the disordered lattice, ions of different charge are randomly distributed along lattice cites). In the sc2 lattice, we have $n_1 = n_2$, while in a disordered binary bcc lattice the n_1/n_2 ratio can be arbitrary. In Igarashi & Iyetomi (2003) elastic coefficients were calculated by taking the second derivative of the Madelung energy, while the Madelung energy was defined as a minimal energy of around 1000 ions in the cubic cell (the minimization procedure was iterated until the relative variance of the energy reached 10^{-6}).

It is well known that the linear mixing (lm) rule has been successfully applied for calculating thermodynamic properties of classical Coulomb mixtures (e.g. Chabrier & Ashcroft 1990; Potekhin, Chabrier & Rogers 2009; Chugunov 2012) and the electrostatic energy of the sc2 lattice Kozhberov & Baiko (2015). Here we try to check its validity for the elastic moduli of Coulomb lattices. According to this rule, the modulus c_{44} of any (ordered and disordered) binary lattice is equal to

$$c^{\rm lm}_{44} \equiv c^{Z_1}_{44}\left(\frac{n_1}{n} + \frac{n_2}{n}\alpha^{5/3}\right)\left(\frac{n_1}{n} + \frac{n_2}{n}\alpha\right)^{1/3}\,, \tag{14}$$

where $c^{Z_1}_{44}$ is the elastic modulus of the one-component lattice which consist of ions with the charge number Z_1. For the sc2 lattice,

$$c^{\rm lm}_{44,\rm sc2} = 0.18276965n\frac{Z_1^2e^2}{2^{4/3}a}(1 + \alpha^{5/3})(1 + \alpha)^{1/3}\,. \tag{15}$$

Other elastic moduli can be calculated in the same way.

Thus the elastic coefficients of the binary bcc lattice with $n_1 = n_2$ can be calculated analytically from the electrostatic energy of the deformed crystal via linear mixing rule and obtained from numerical simulations. For several values of α the coefficients c_{44} are presented in Table 2. The results of Igarashi & Iyetomi (2003) are labelled as $c^{\rm dis}_{44}$. Igarashi & Iyetomi (2003) investigated lattices with $\alpha \le 13$ while we restrict ourselves to $\alpha = 3$, because (as shown by Kozhberov & Baiko 2012) the sc2 lattice is stable with respect to the small oscillations of ions around their equilibrium positions at $\alpha < 3.6$ (similar result was obtained latter in Kalman et al. 2014 from molecular dynamics).

One can see a noticeable difference between c_{44} for ordered and disordered binary bcc lattices, especially at high α. The linear mixing rule does not allow one to calculate this elastic coefficient with appropriate precision. The same is true for other elastic moduli ($s^{\rm xxxx}$ and $s^{\rm xxyy}$) of the sc2 lattice.

4 EFFECTIVE SHEAR MODULUS

The matter in a neutron star crust is often assumed to be polycrystalline (e.g. Horowitz & Kadau 2009; Caplan et al. 2018). Then the crust consist of randomly oriented crystals, and it is convenient to use an effective shear modulus $\mu_{\rm eff}$. However, the question of how to determine $\mu_{\rm eff}$ remains open (Kobyakov & Pethick 2015).

At first, we use the way which is the most common in theory of degenerated stars, and define the effective shear modulus as

Table 3. Values of $\mu_{\rm eff}$ in units of $nZ_1^2e^2/a$ of the binary bcc lattice.

α	4/3	2	3
$\mu_{\rm eff}^{\rm sc2}$	0.164 451	0.285 482	0.544 639
$\mu_{\rm eff}^{\rm dis}$	0.164	0.284	0.542
$\mu_{\rm eff}^{\rm lm,sc2}$	0.164 439	0.285 44	0.544 853
$\mu_{\rm eff,m}^{\rm sc2}$	0.139 547	0.282 088	0.517 677
$\mu_{\rm eff,m}^{\rm dis}$	0.138	0.284	0.542
$\mu_{\rm eff,m}^{\rm lm,sc2}$	0.128 027	0.222 235	0.424 206

an average of the shear stiffness over all possible wavevectors and for polarization vectors perpendicular to the wave vector, which is equivalent to the Voigt average (see details in Ogata & Ichimaru 1990; Baiko 2011, for the one-component crystals). In our notations,

$$\mu_{\rm eff} \equiv \frac{1}{5}(s^{\rm xxxx} - s^{\rm xxyy} + 3s^{\rm xyxy} - p')\,. \tag{16}$$

For the sc2 lattice, we have $s_{\rm sc2}^{\rm xyxy} = -s_{\rm sc2}^{\rm xxxx}/2$, $s_{\rm sc2}^{\rm xxxx} + 2s_{\rm sc2}^{\rm xxyy} = 2p'$, and $\tilde{p}' = \xi'/3$. Then $\mu_{\rm eff}^{\rm sc2}$ depends only on the Madelung constant (Chugunov 2019),

$$\mu_{\rm eff}^{\rm sc2} = -\frac{2}{15}\xi_{\rm sc2}\frac{nZ_1^2e^2}{a}$$
$$= \left(0.0465669(1+\alpha^2) + 0.0263234\alpha\right)\frac{nZ_1^2e^2}{a}\,. \tag{17}$$

For the bcc lattice

$$\mu_{\rm eff}^{\rm bcc} = -\frac{2}{15}\xi_{\rm bcc}n\frac{Z^2e^2}{a}$$
$$= 0.1194572n\frac{Z^2e^2}{a} = 0.4852310n\frac{Z^2e^2}{2a_1}\,, \tag{18}$$

which agrees with the results of Baiko (2011).

According to Kozhberov & Baiko (2015), the linear mixing rule can be successfully used to calculate the electrostatic energy of the sc2 lattice $\left(U_{\rm M}^{\rm lm}\right)$. The ratio of the exact $U_{\rm M}$ to $U_{\rm M}^{\rm lm}$ lies between 0.999 843 at $\alpha \approx 1.826\,19$ and 1.000 94 at $\alpha = 3.6$. Hence the linear mixing rule can also be successfully applied to determine the effective shear modulus defined by equation (16),

$$\mu_{\rm eff}^{\rm lm,sc2} = 0.119457n\frac{Z_1^2e^2}{2^{4/3}a}(1+\alpha^{5/3})(1+\alpha)^{1/3}\,. \tag{19}$$

For some values of α, the quantities $\mu_{\rm eff}^{\rm sc2}$ and $\mu_{\rm eff}^{\rm lm,sc2}$ are presented in Table 3.

The effective shear modulus of the disordered binary bcc lattice obtained by Igarashi & Iyetomi (2003) is denoted in Table 3 as $\mu_{\rm eff}^{\rm dis}$. The difference between $\mu_{\rm eff}$ for the ordered and disordered lattices is insignificant and does not exceed computational errors.

There are some other ways to determine the effective shear modulus of polycrystals. For the bcc lattice, they are summarized by Kobyakov & Pethick (2015). Among all of these ways we focus on the effective medium theory based on a multiple scattering formalism (e.g. Zeller & Dederichs 1973; Robbins et al. 1988). According to this theory, the effective elastic modulus of a one-component cubic crystal can found from the equation,

$$3\mu_{\rm eff,m}^2 - s^{\rm xyxy}\mu_{\rm eff,m} - (s^{\rm xxxx} - s^{\rm xxyy} - p')s^{\rm xyxy} = 0\,, \tag{20}$$

where we take into account that the dominated contribution to the pressure comes from degenerated electrons (Kobyakov & Pethick 2015). For the bcc lattice we obtain

$$\mu_{\rm eff,m}^{\rm bcc} = 0.377786n\frac{Z^2e^2}{2a_1} = 0.0930057n\frac{Z^2e^2}{a}\,. \tag{21}$$

For the sc2 lattice and several values of α, the values of $\mu_{\rm eff,m}^{\rm sc2}$ are given in Table 3. For this definition of the effective shear modulus, exact results are inconsistent with the results of numerical simulations (Igarashi & Iyetomi 2003; $\mu_{\rm eff,m}^{\rm dis}$ in Table 3) and with the results obtained from the linear mixing rule ($\mu_{\rm eff,m}^{\rm lm,sc2}$ in Table 3). The difference between $\mu_{\rm eff}^{\rm sc2}$ and $\mu_{\rm eff,m}^{\rm sc2}$ is appreciable. The $\mu_{\rm eff}^{\rm sc2}/\mu_{\rm eff,m}^{\rm sc2}$ ratio changes non-monotonically with α as plotted in Fig. 1. At $\alpha = 1$ it is equal to 1.284 41, which is the maximum. The minimum is reached at $\alpha \approx 2.29$ and equals 1. At $\alpha = 3.6$ we have $\mu_{\rm eff}^{\rm sc2}/\mu_{\rm eff,m}^{\rm sc2} \approx 1.16175$. Notice that at $\alpha = 2$ and $\alpha = 3$ for the disordered crystal both methods give the same result ($\mu_{\rm eff}^{\rm dis} = \mu_{\rm eff,m}^{\rm dis}$).

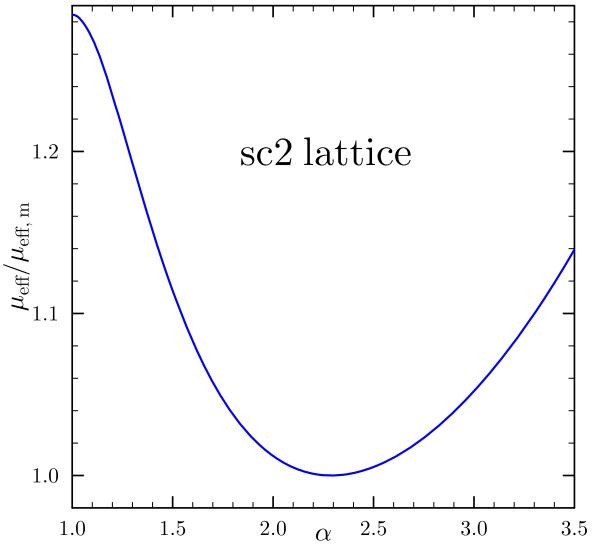

Figure 1. The ratio of the $\mu_{\rm eff}$ values calculated by different methods for the sc2 lattice.

5 SCREENING CORRECTIONS

Using the same method as in the previous sections, we can calculate the elastic coefficients of the one-component bcc Coulomb crystal with polarized electron background. The polarization correction to the electrostatic energy was derived by Baiko (2002; see his equation 9). The only difference from the uniform case is that the screening parameter $\kappa_{\rm TF}a$ also depends on volume changes during stretches along edges of the main lattice cube; for degenerate electrons and one-component lattices $\kappa_{\rm TF}a \approx 0.185Z^{1/3}(1+x_{\rm r}^2)^{1/4}/x_{\rm r}^{1/2}$, where $x_{\rm r}$ is the electron relativity parameter.

Screening corrections (scr) to the electrostatic pressure and effective shear modulus of the bcc lattice are

$$p^{\rm scr} = \frac{\eta}{3}\frac{x_{\rm r}^2}{1+x_{\rm r}^2}(\kappa_{\rm TF}a)^2n\frac{Z^2e^2}{a}, \tag{22}$$

$$c_{44}^{\rm scr} = -0.041198(\kappa_{\rm TF}a)^2n\frac{Z^2e^2}{a}, \tag{23}$$

$$\mu_{\rm eff}^{\rm scr} \approx -0.027662(\kappa_{\rm TF}a)^2n\frac{Z^2e^2}{a}$$
$$= \frac{4\eta}{15}(\kappa_{\rm TF}a)^2n\frac{Z^2e^2}{a}\,, \tag{24}$$

where $\eta = -0.103\,732\,3337$ is the screening correction to the electrostatic energy. These results agree with and improve the results of Baiko (2015), where the screening corrections to the Coulomb crystal elastic moduli were systematically studied for the first time. Also, they were studied by Horowitz & Hughto (2008) via molecular dynamics simulations for the bcc Coulomb crystal. At $\kappa_{\rm TF}a \approx 0.5705$ and $T = 0$, it was obtained that the effective shear modulus defined by equation (16) equals $0.1108nZ^2e^2/a$. Our calculations give $\mu_{\rm eff} \approx 0.1105nZ^2e^2/a$, so that the agreement is quite well. Note that Robbins et al. (1988) studied the screening corrections for the systems with non-degenerate electron background. For that reason, the direct comparison with our results is not possible.

6 BINARY FACE-CENTRED CUBIC LATTICE

We have also considered the binary fc2 lattice. In this case $n_2 = 3n_1$. The ions with lower number density have the change number Z_1 (see fig. 3 from Chamel & Fantina 2016; where this lattice is called 'the sc2 lattice'). In the elementary cell ions with Z_1 located on corners of the cube, ions with Z_2 are centred on its faces. The electrostatic energy of the fc2 lattice is

$$U_{\rm M} = -N\frac{Z_1^2e^2}{2a_1}\xi'_{\rm fc2} = -N\frac{Z_1^2e^2}{a}(0.138600677 + 0.1707354535\alpha + 0.5865374846\alpha^2)\,, \quad (25)$$

and $\xi'_{\rm fc2} = 2(2\pi/3)^{1/3}\xi_{\rm fc2}$. For the first time this expression was obtained by Jog & Smith (1982); here it is presented with improved accuracy.

The consideration of the same deformations as for the sc2 lattice in Section 3 gives

$$\tilde{p}'_{\rm fc2} = \xi'_{\rm fc2}/3 \quad (26)$$

$$\tilde{s}^{\rm xxxx}_{\rm fc2} = 0.16484692 - 1.27801856\alpha - 0.78347781\alpha^2\,, \quad (27)$$

$$\tilde{s}^{\rm xxyy}_{\rm fc2} = -0.31886491 + 0.34774851\alpha - 0.60884623\alpha^2\,, \quad (28)$$

$$\tilde{s}^{\mathbf{xyxy}}_{\rm fc2} = -\tilde{s}^{\rm xxxx}_{\rm fc2}/2\,. \quad (29)$$

For the fcc lattice we obtain $\tilde{p}'_{\rm fcc} = -1.528\,287\,358$, $\tilde{s}^{\rm xxxx}_{\rm fcc} = -1.896\,649\,45$, $\tilde{s}^{\rm xxyy}_{\rm fcc} = -0.579\,962\,63$, and $\tilde{s}^{\rm xyxy}_{\rm fcc} = 0.948\,324\,73$, then $-\tilde{p}'_{\rm fcc} + \tilde{s}^{\rm xxxx}_{\rm fcc} - \tilde{s}^{\mathbf{xxyy}}_{\rm fcc} = 0.211\,600\,53$. The latter value is in good agreement with the result of Fuchs (1936), who obtained 0.2115. The values $\tilde{s}^{\rm xxxx}_{\rm fcc}$ and $\tilde{s}^{\rm xxyy}_{\rm fcc}$ were not presented by Fuchs (1936). According to Fuchs (1936), $\tilde{s}^{\rm xyxy}_{\rm fcc} = 0.9479$, which also agrees with our result. The one-component fcc lattice was also studied by Robbins et al. (1988).

From equations (26–29) the effective shear modulus of the fc2 lattice defined by equation (16) is

$$\mu^{\rm fc2}_{\rm eff} = -\frac{2}{15}\xi_{\rm fc2}n\frac{Z_1^2e^2}{a} = n\frac{Z_1^2e^2}{a}(0.01848009 + 0.02276473\alpha + 0.07820500\alpha^2)\,. \quad (30)$$

The effective shear modulus of the fcc lattice ($\alpha = 1$) is equal to

$$\mu^{\rm fcc}_{\rm eff} = -\frac{2}{15}\xi_{\rm fcc}n\frac{Z^2e^2}{a} = 0.11944982n\frac{Z^2e^2}{a}\,. \quad (31)$$

Data from Fuchs (1936) gives the same value. The difference between $\mu^{\rm bcc}_{\rm eff}$ and $\mu^{\rm fcc}_{\rm eff}$ is small but only for the chosen definition of $\mu_{\rm eff}$, because the difference between the Madelung constants of these lattices is small. In this case

$$\mu^{\rm fcc}_{\rm eff,m} = 0.0901087n\frac{Z^2e^2}{a}\,. \quad (32)$$

Note that the bcc lattice can be turned into the fcc lattice by continuous deformation (Baiko & Kozhberov 2017).

According to the linear mixing rule, $\mu_{\rm eff}$ of the binary fcc lattice is

$$\mu^{\rm lm,fc2}_{\rm eff} = 0.11944982n\frac{Z_1^2e^2}{2^{8/3}a}(1+3\alpha^{5/3})(1+3\alpha)^{1/3}\,. \quad (33)$$

Our analysis of the phonon spectrum shows that the fc2 lattice is stable at $0.66 \le \alpha \le 1.36$ (step over α equals 0.02; see Kozhberov 2018, for details). This result agrees with the limits of stability of the fc2 lattice obtained independently by Kalman et al. (2014): $0.661 \le \alpha \le 1.368$. For this range of α, the $\mu^{\rm lm,fc2}_{\rm eff}/\mu^{\rm fc2}_{\rm eff}$ ratio always ranges between 1 and 1.002. As for the sc2 lattice, the elastic moduli $s^{\rm xxxx}$, $s^{\rm xxyy}$, and $s^{\rm xyxy}$ of the fc2 lattice cannot be calculated using the linear mixing rule.

7 DISCUSSION AND CONCLUSIONS

We discuss elastic properties of the binary Coulomb crystals. Our results demonstrate that the Voigt averaged effective shear modulus calculated for ordered crystals well agrees with the numerical results for disordered crystals. It is also shown that the linear mixing rule can be applied to calculate $\mu_{\rm eff}$, providing thus a simple approach to estimate effective shear modulus for neutron star crust and crystallized white dwarf core. It should be stressed that the linear mixing rule is inapplicable to other elastic moduli of the sc2 and fc2 lattices. The possible explanation may be that $s^{\rm xxxx}$, $s^{\rm xxyy}$, and $s^{\rm xyxy}$ related with properties of the separated parts of the crystal and not with the whole one. The same concern the difference between our results and results obtained in Igarashi & Iyetomi (2003). This discrepancy can be a great motivation for the future numerical work. Furthermore, it is shown that the elastic constants for sc2 and fc2 lattices have additional coupling, which does not follow from their symmetry: $s^{\rm xxxx} = -2\,s^{\rm xyxy}$.

The Voigt average is not the only approach to estimate the effective shear modulus of the polycrystalline matter (see Section 4), in particular it can be estimated according to equation (20). Here we show that the resulting $\mu_{\rm eff,m}$ differs for ordered and disordered crystals. For ordered crystals ratio between $\mu_{\rm eff}$ and $\mu_{\rm eff,m}$ is less than 30 per cent for any possible charge ratio. In addition, the linear mixing rule does not allow to calculate $\mu_{\rm eff,m}$ with the appropriate for the practical use precision. Applying obtained results we can conclude that for the binary systems in degenerated stars it may be better to use the Voigt averaged effective shear modulus because it contains less uncertainties.

For astrophysical purposes it is convenient to rewrite $\mu^{\rm sc2}_{\rm eff}$ and $\mu^{\rm fc2}_{\rm eff}$ as a function of concentration of electrons $n_{\rm e} \equiv \bar{Z}n$, where $\bar{Z}$ is the averaged ion charge in the crystal. For the sc2 lattice $\bar{Z} = (Z_1 + Z_2)/2$ and for the fc2 lattice $\bar{Z} = (Z_1 + 3Z_2)/4$ then,

$$\mu^{\rm sc2}_{\rm eff} = \frac{n_{\rm e}}{a_{\rm e}}\frac{4(\bar{Z}e)^{2/3}}{(1+\alpha)^2} \times \left(0.0465669(1+\alpha^2) + 0.0263234\alpha\right)\,, \quad (34)$$

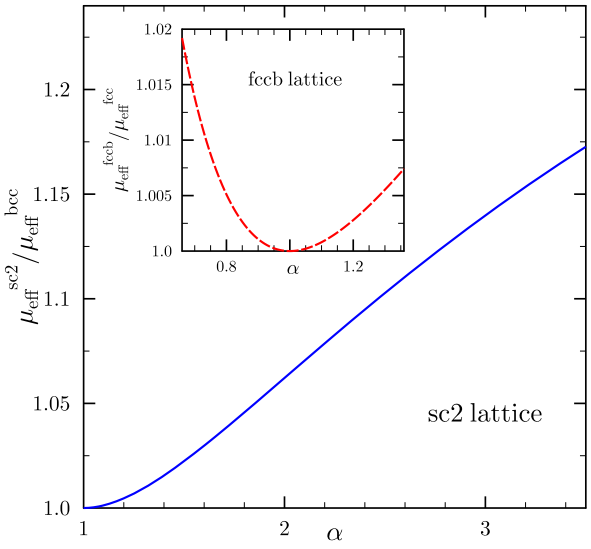

Figure 2. The effective shear modulus of binary Coulomb crystals.

$$\mu_{\rm eff}^{\rm fc2} = \frac{n_{\rm e}}{a_{\rm e}}\frac{16(\bar{Z}e)^{2/3}}{(1+3\alpha)^2} \times \left(0.01848009 + 0.02276473\alpha + 0.07820500\alpha^2\right), \quad (35)$$

where $a_{\rm e} \equiv (4\pi n_{\rm e}/3)^{-1/3}$. Ratios $\mu_{\rm eff}^{\rm sc2}/\mu_{\rm eff}^{\rm bcc}$ and $\mu_{\rm eff}^{\rm fc2}/\mu_{\rm eff}^{\rm fcc}$ at fixed $n_{\rm e}$ are plotted in Fig. 2 as a function of α, where $\mu_{\rm eff}^{\rm bcc}$ and $\mu_{\rm eff}^{\rm fcc}$ are the effective shear modulus of one-component crystals of ions with charge $\bar{Z}e$.

For the stable lattices changes of ratios in Fig. 2 are small. For the fully ionized carbon–oxygen mixture in white dwarf envelopes they are equal to 1.011 41 for the sc2 lattice and 1.006 56 (at $\alpha = 4/3$, 25 per cent C, and 75 per cent O) or 1.008 73 (at $\alpha = 3/4$, 75 per cent C, and 25 per cent O) for the fc2 lattice. According to the linear mixing rule the difference between $\mu_{\rm eff}$ of the disordered carbon–oxygen crystal and $\mu_{\rm eff}$ of the one-component crystal with the ion charge $\bar{Z}e$ and at the same $n_{\rm e}$ does not exceed a few per cent.

The similar situation takes place for ^{56}Fe + ^{62}Ni ($\mu_{\rm eff}^{\rm sc2}/\mu_{\rm eff}^{\rm bcc} \approx 1.000\,77$ at $\alpha = 14/13$) and ^{80}Ni + ^{120}Mo ($\mu_{\rm eff}^{\rm sc2}/\mu_{\rm eff}^{\rm bcc} \approx 1.022\,37$ at $\alpha = 1.5$) binary sc2 lattices. Formation of these crystals in the neutron star crust was predicted in Chamel & Fantina (2016). They are resistant to the separation into two one-component bcc crystals.

The difference between $\mu_{\rm eff}^{\rm sc2}$ and $\mu_{\rm eff}^{\rm bcc}$ is more important for the oxygen–iron and oxygen–nickel mixtures. For these mixtures $\alpha = 3.25$ and $\alpha = 3.5$, respectively, and they could form a sc2 lattice. At $\alpha = 3.25$ $\mu_{\rm eff}^{\rm sc2}/\mu_{\rm eff}^{\rm bcc} \approx 1.156\,75$, while at $\alpha = 3.5$ $\mu_{\rm eff}^{\rm sc2}/\mu_{\rm eff}^{\rm bcc} \approx 1.172\,62$. However possibility of formation these crystals in degenerate stars should be checked.

Hence, for the binary crystal mixtures in neutron star crust using the effective shear modulus of a one component Coulomb crystal with averaged charge seems to be a good assumption. For compounds with more than two types of ions in the elementary cell, it should be checked both analytically (for instance, by the same method which was used in the current paper) and numerically.

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