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To cite this article: D O Gericke et al 2010 J. Phys.: Conf. Ser. 220 012001

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Structural Properties of Warm Dense Matter

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Abstract. We investigate the structure in warm dense matter by ab initio simulations and classical fluid equations. This comparison yields valuable information on the system properties such as effective ion-ion interactions and charge states. Extensions to systems with multiple ion species are discussed and the limits of reduced descriptions are demonstrated. The structural information is then used to predict the signal strength in x-ray scattering experiments which, in turn, can be used as diagnostics for warm dense fluids. Here, we need to consider the inelastic feature due to the dynamic response of free electrons as well as the elastic (Rayleigh) peak related to the static ion structure. In a last example, we apply ab initio simulations to calculate the ionic structure in highly excited graphite close to melting.

1. Introduction
Warm dense matter (WDM) is a state with densities comparable to solids and temperatures of a few electron volts. These conditions naturally occur, e.g., in the crusts of neutron stars, the main volume of brown dwarfs, in the interior of giant gas planets [1, 2, 3, 4] as well as the center of earth-like planets [5]. In the laboratory, WDM states are created, at least as a transient state, during the interaction of intense lasers or particle beams with solids [6]. Special interest is thus directed to the properties of WDM when designing targets for inertial confinement fusion. In indirectly driven targets, WDM states are found in the converters, the walls of the hohlraum, and the hydrogen core during the compression phase [7, 8]. Due to reduced shock-heating of the hydrogen, WDM is particularly prominent in the pre-compressed core of targets for fast ignition, a more energy efficient inertial confinement fusion scheme with higher gains [9, 10].

In the region of WDM, the correlation, the electron Fermi and the effective ionization energies are all of the same order of magnitude making it intrinsically a strongly correlated quantum system. The challenges for a theoretical description are therefore similar to those arising when considering such diverse systems as ultra-cold atoms in traps, electrons in high-temperature superconductors and nuclear matter [11]. In contrast to the other systems, WDM has two distinct species: the strongly coupled but classical ions and the partially degenerate electrons which can be affected by correlations as well. The strength of the ion-ion correlations and the electron degeneracy can be estimated by the parameters [12]

\[
\Gamma_{ii} = \frac{Z^2_i e^2}{a_i k_B T_i} \quad \text{and} \quad n_e A_e^3 = n_e \left( \frac{2\pi \hbar^2}{m_e k_B T_e} \right)^{3/2},
\]

where \(a_i = (3/4\pi n_i)^{1/3}\) is the mean inter-ionic distance. The classical coupling parameter \(\Gamma\) gives the ratio of the mean potential to the kinetic energies. Of course, a similar parameter can
be defined for the electrons, but one has to replace the classical thermal energy, that is $k_B T$, by the appropriate energy of the quantum system which becomes the Fermi energy for highly degenerate systems. Due to high electron densities and temperatures, the electrons are however mainly weakly to moderately coupled in WDM.

Whereas degeneracy in weakly coupled systems can be easily treated, strongly coupled systems represent a challenge for a theoretical description. The definitions (1) demonstrate that strong coupling may be created by either low temperatures or high enough particle densities. An extreme example for the first approach are ultra-cold plasmas [13, 14, 15] which are created by laser-ionization of ultra-cold gases in magneto-optical traps. As the laser energy considerably heats the electrons, one can describe the electron background as a nondegenerate and weakly coupled fluid [16]. The ions, however, show significant correlation effects: the laser ionization suddenly changes the potential energy landscape in the system and, as a result, the ions build a structure according to the new forces. This releases large amounts of potential energy which increases the ion temperature by orders of magnitude to states with $1 < \Gamma < 5$ [17, 18, 19]. Further laser cooling of the ions can even increase the coupling enough to create Coulomb crystals [20] similar to those known in dusty plasmas [21, 22].

Although the effects of strong coupling can be studied in detail in ultra-cold and dusty plasmas, the ions in such systems can be mainly described as classical one component plasmas (OCP) and lack the combination of partially degenerate electrons and strongly coupled ions. This mutual influence of quantum behavior and strong interactions is only found in the region of WDM with its high densities and moderate temperatures. Again, the degenerate electron fluid alone may be sufficiently described by the random phase approximation (RPA) or its extensions considering weak binary collisions [12]. Moreover, effective approaches based on integral equations [23, 24] exist to describe strongly coupled plasmas in the classical domain. For Coulomb systems with coupling strength up to $\Gamma = 100$, these approximate models have been shown to yield results similar to direct simulations [25]. However, integral equations as well as molecular dynamics and Monte Carlo simulations treat systems with known interactions. In WDM, the effective ion-ion interactions and the electronic response have to be self-consistently determined as both strongly influence each other. This fact becomes particularly clear when considering the charge state of the ions: due to the strong interactions with free electrons and other ions, thermally stable bound states can vanish and move into the continuum (as the conduction electrons in metals); moreover, a precise distinction between bound and free states might not be possible as the binding and correlation energies are often of the same order and, thus, the bound states become highly resonant.

The demand for highly accurate theoretical description of WDM can nowadays not be met by an approach based on Green’s functions. We therefore apply density functional molecular dynamics (DFT-MD) simulations as an alternative method. DFT-MD fully meets the demands for a theoretical description of WDM as the electrons are treated with density functional theory (full quantum mechanics) and the ion positions are moved under the influence of forces that include the direct ion-ion as well as the electron-ion contributions. The latter are, of course, determined self-consistently from the DFT electron configuration. We then use comparisons with more approximate classical hypernetted chain (HNC) calculations to obtain valuable information on ion-ion interactions and the charge states. Both methods are applied to lithium, beryllium and CH as these materials were recently investigated experimentally in the WDM region [26, 27, 28, 29, 30]. We find that most materials can be described well by a linearly screened Coulomb potential which can be improved by an additional repulsive potential. For beryllium, we find a stable charge state of $Z=2$ which is consistent with measurements and can also rule out suggested quantum-potentials. Extensions to mixtures show that an approximative treatment based on one component calculations [31] works for weakly coupled ions, but fails for strong coupling. Finally, we apply the DFT simulation technique to highly excited carbon in
the solid phase.

2. Determining the Ion Structure in WDM

We will use a combination of *ab initio* simulations and integral equations derived in fluid theory (HNC approach) to obtain information on the ionic structure, the effective ion-ion interaction and the electron configuration in WDM. While the full quantum simulations serve as a benchmark, the HNC calculations are matched with the results to determine the effective interactions. Such reduced models are urgently needed for practical applications as the DFT-MD simulations are computationally very expensive. For instance, for plasma diagnostics by means of x-ray scattering [32, 33, 34], one needs the ion structure for many parameters as the density and temperature are obtained by matching the experimental spectrum by changing the input density and temperature in the theoretical calculation. Such a diagnostics method would not be applicable if DFT-MD simulations with run times of days/weeks would be used for every possible set of system parameters.

2.1. DFT-MD simulations

We apply Born-Oppenheimer DFT-MD simulations, that is DFT for the electrons and classical MD for the ions where the electronic configuration is updated at every step. In more detail: the Hohenberg-Kohn theorem [35, 36] proves that the electron ground state density contains sufficient information to fully determine the electron subsystem and the electron wave functions are not needed. This freedom is used by the Kohn-Sham ansatz that connects the fully interacting electron system with its noninteracting counterpart by requesting that the electron density is kept [37]. Of course, this requires that the noninteracting electrons are considered in an additional external potential which is still to be determined. The electron density can then be derived from the generalized Schrödinger equation for single electrons

$$\left[-\frac{1}{2}\nabla^2 + V_{KS}^{\sigma}(r)\right] \psi_{i}^{\sigma}(r) = \varepsilon_{i}^{\sigma} \psi_{i}^{\sigma}(r).$$

(2)

The Kohn-Sham potential $V_{KS}$ can be decomposed as

$$V_{KS}^{\sigma}(r) = V_{ext}(r) + V_{H}[n] + V_{xc}^{\sigma}[n^{\uparrow}, n^{\downarrow}],$$

(3)

where the first term is the real external potential created by the ions, the second term is the Hartree field and the last contribution is the exchange-correlation potential. As this last term contains the full many-body physics, it is not fully known and, thus, is the only point where the DFT calculations become approximate. However, one can derive powerful approximations for the exchange-correlation potential $V_{xc}$. The easiest is the local density approximation [36] which is further improved by the generalized gradient approximation. The latter is used for the presented results by applying the Perdew-Burke-Ernzerhof type [38] for the exchange-correlation potential.

The original DFT is a pure ground state calculation and thus not applicable in WDM as thermal and Fermi energies are comparable. Thus, the Fermi distribution deviates from a step function and a $T = 0$ treatment is not applicable. Temperature effects in the electron component can be included by using the Mermin functional [39] that populates the energy eigenstates by the real temperature-dependent Fermi function.

For our DFT-MD simulations we use the VASP package [40, 41, 42] that implements density functional theory and combines it with a MD solver for the ions: for a given ion configuration, the Kohn-Sham equations are solved and the energy levels are then populated according to the electron Fermi distribution. From the given electron configuration, electron-ion forces are derived and the ions are moved in a classical MD step. Then the loop is started again and a
results from density functional molecular dynamics (DFT-MD) simulations of hydrogen with a density of \( \rho = 3.7 \text{ g cm}^{-3} \) and a temperature of \( T = 4000 \text{ K} \). Shown are the hydrogen nuclei (cyan spheres) and an iso-surface of the electron density (red). Here, hydrogen is pressure ionized and, therefore, is in an atomic-metallic phase.

Figure 2. Same as left figure, but for a lower density of \( \rho = 0.2 \text{ g cm}^{-3} \) and with an additional iso-surface shown in grey. Clearly, hydrogen is here in the molecular phase.

new electron density is calculated for the new ion configuration. It is important to notice that the electrons are considered to instantaneously react on the new ion field and that the DFT calculations are done at every MD step (Born-Oppenheimer DFT-MD).

Initially, the ions are not in equilibrium and one has to allow for an equilibration phase before extracting the physical properties. During this time, the ions build up correlation energy which, depending on their initial configuration, can considerably change their temperature. The ion temperature is then controlled via a Nose-Hoover thermostat [43]. Combined with the Mermin functional, we can thus consider both electron and ion distributions at a given finite temperature.

We have performed the simulations for 128 or 256 nuclei while treating all electrons as valence. For the fluids considered, we can use the Gamma point only to sample the Brillouin zone. The VASP package uses a plane wave expansion to solve the Kohn-Sham equations (2). To include all bound states and fully sample the Fermi distribution, we use a rather high cutoff energy of 800 eV. This requires roughly five times the number of bands as for ground state calculations which makes the calculations computationally even more expensive and also limits the temperature that can be considered. The ions are moved with a time step of 0.4 fs to fully resolve the motion under strong fields from other ions. When extracting the structural information, we average over more than 1000 different configurations (ion steps) to counter the bad statistics due to the small systems size.

Figures 1 and 2 show snapshots from DFT-MD simulations of hydrogen at two densities. Although the information that can be extracted from such pictures is rather limited, one can already observe that the two systems are in quite different states: while the electron density in the first figure fills the whole space, the electrons are localized around the ions for the second
case and the ions are paired here. We can therefore conclude that Fig. 1 shows hydrogen in the metallic phase whereas hydrogen is a molecular fluid for the conditions of Fig. 2.

2.2. HNC calculations

To extract more information from the DFT-MD simulations, we compare the results with data from hypernetted chain (HNC) calculations [24]. Important quantities are the ionic pair distribution $g_{ii}(r)$ and the ion-ion structure factor $S_{ii}(k)$. As the HNC scheme uses a given ion-ion pair potential, the comparison with DFT-MD simulations assesses the quality of the potential used.

HNC calculations are based on the Ornstein-Zernike relation that defines the direct correlation functions $c(r)$ as a functional of the total correlation function $h(r) = g(r) - 1$. Considering multi-component systems, we have in Fourier space [23]

$$h_{ab}(k) = c_{ab}(k) + \sum_c n_c c_{ac}(k) h_{cb}(k). \quad (4)$$

As this equation is a definition, it can be considered to be exact. However, we need a closure relation to fully determine $h(r)$ and $c(r)$ which can be obtained by a cluster expansion [44, 45]

$$g_{ab}(r) = \exp[-\beta V_{ab}(r) + h_{ab}(r) - c_{ab}(r) + B_{ab}(r)]. \quad (5)$$

Here, $B(r)$ is the bridge function that is not exactly known. Therefore, different approximations to the closure relation (5) have been tested against direct MD or MC simulations (see, e.g., Ref. [25]). It turns out that the HNC approximation which neglects the bridge function, that is $B(r) = 0$, yields quite good results for Coulomb-like systems. Thus, we adopt this approach in the following. An even faster approach is given by the mean spherical approximation (MSA) for charged hard spheres which can be solved analytically [46, 47]. Interestingly, this yields also rather good results for Coulomb systems up to high coupling strength [48].

Figure 3 shows an example for the pair distribution $g(r)$ in a mixture of two ion species where all particles interact via pure Coulomb forces (no screening). Typical for the structure in strongly coupled systems are the correlation hole at small separations and the following maxima and minima. As the aluminium ions are more highly charged, they show a more pronounced

![Figure 3](image1.png)

**Figure 3.** Partial pair distributions for a mixture of aluminium and lithium ions with $n_{Al} = n_{Li} = 7.6 \times 10^{22} \text{cm}^{-3}$ and $T = 1 \text{eV}$. The ion charge states are $Z_{Al} = 3$ and $Z_{Li} = 1$.

![Figure 4](image2.png)

**Figure 4.** Partial structure factors for the same system as in Fig. 3. Note that the cross term $S_{AlLi}$ lacks unity in the definition and, thus, has a different behaviour at large $k$. 


structure. This component is also mainly responsible for the Al-Li and the Li-Li structure as the aluminium ions imprint their configuration on the lithium ions [49].

Figure 4 shows the partial ion-ion structure factors defined as

\[ S_{ab}(k) = \delta_{ab} + \sqrt{n_an_b} \int dr [g_{ab}(r) - 1] \exp(ikr) \]  

for the same case. Again, the Al-Al term shows the most structure. In contrast to the pair distribution, the Li-Li structure factor appears almost without structure. Here, we observe a competing effect of correlations and screening: although pure Coulomb interactions are applied the (nonlinear!) screening of the Coulomb forces by the other ion species is self-consistently included in the HNC scheme. This becomes particularly pronounced at small \( k \). Indeed, the structure factor at \( k = 0 \) directly shows the strength of screening as an unscreened one component plasmas has \( S_{ii}(0) = 0 \). Thus, the value of \( S_{LiLi}(k) \) at small \( k \) indicates strong screening not weak direct forces. The quite different behaviour of \( S_{AlLi}(k) \) results mainly from the fact that its definition does not include unity as the Kronecker symbol in Eq. (6) vanishes for \( a \neq b \).

3. Quantum Potentials, Effective Ion-Ion Interactions and Ion Charge States

First we evaluate the ability of the multi-component HNC approach to describe electron-ion systems. Then we use the comparison of the ionic structure obtained by DFT-MD and HNC to extract information on the effective ion-ion interaction and the electronic configuration.

3.1. Testing Electron-Ion Quantum Potentials

The HNC equations (4) and (5) are formulated for multi-component systems. They could also be used to model electron-ion systems and thus go beyond linear screening. However, the HNC scheme is a classical approach and neglects the quantum nature of the electrons. Technically, this results in too high electron densities near the ion core and too high electron-electron distributions for degenerate systems.

These issues might be resolved by the use of quantum pseudo-potentials for the electron-ion and electron-electron interactions that mimic the quantum behaviour in classical calculations. Different forms of such potentials have been suggested or derived [50, 51]. The application of such potentials is usually limited to weakly coupled and weakly degenerate plasmas making their application in calculations for WDM highly questionable. However, recent experimental results from x-ray Thomson scattering on warm dense beryllium [28] suggested that the ultra-weak Klimontovich-Kraeft (KK) potential (see Ref. [49] for its definition) is applicable here. Here, the results from HNC calculations using the KK potential should be compared to DFT-MD data to justify or falsify such a statement.

Figure 5 shows a comparison of the DFT-MD data with HNC results using the KK potential and different charge states of the ions. Clearly, the HNC results cannot match the DFT-MD data even for the wide range of ion charge states considered. The ions always seem to be too strongly correlated which results from the fact that the KK potential is very weak and thus screening of the ion-ion potential is underestimated [49]. Although it is less pronounced, the comparison for the ionic structure factors in Fig. 6 indicates the same. Similar statements can be made for other quantum pseudo-potentials as well [52]. We thus can conclude that indeed a classical treatment using the KK potential cannot be applied for the WDM condition considered here and the low intensities of the elastic scattering feature reported in Ref. [28] must have a different reason than the ion structure.

3.2. Extracting the Ion Charge State from DFT-MD Simulations

In contrast to HNC scheme using the KK potential, the DFT-MD data for warm dense beryllium and other materials can be matched by HNC calculations that treat only the ions explicitly and
consider the effect of the electrons by using a linearly screened Coulomb potential for the ion-ion interaction (Yukawa model) \[52\]. Even better agreement is obtained if a short range repulsion, that mimics the interactions of the fully occupied shell of core electrons, is added.

We can now adopt this model and match the DFT-MD results by using different charge states for the ions. Fig. 7 shows this comparison for the case of solid-density beryllium tested experimentally \[27, 28\]. We find much better agreement than in Fig. 5 for all charge states considered. As expected, the best match is here found for \(Z = 2\) that is the stable helium-like configuration. Thus, we have here a case with a well-defined charge state as the ionization energy of the 1s electrons is too large to be overcome by either temperature or correlations and the 2s shell is fully ionized as in cold beryllium. Of course, one can also compare the electronic configuration around an ion directly with the bound state density for isolated atoms. For the case presented here, this gives also a charge state of \(Z = 2\) \[53\].

### 3.3. Ion Structure in Moderately to Strongly Coupled Multi-Component Plasmas

Both DFT-MD and HNC are methods that can be naturally applied to systems with multiple ion species. The only problem that arises is purely technical as the computational demands strongly increase with the number of species considered; in particular, for the DFT-MD simulations. Nevertheless, partial ion-ion structure factors for multi-component plasmas are often calculated from one component results using the relation \[54\]

\[
S_{ab}(k) = \delta_{ab} + \frac{\sqrt{n_a n_b}}{n_a + n_b} \frac{Z_a Z_b}{Z_f^2} \left[ S_{ii}^{\text{comp}}(k) - 1 \right].
\]

Here, \(n_a\) and \(Z_a\) are the density and the charge state of the ion species \(a\), respectively, \(Z_f = \sum_a n_a Z_a / \sum_b n_b\) is the average ion charge and \(S_{ii}^{\text{comp}}(k)\) denotes the ion-ion structure factor for a one component system of particles with an average charge \(Z_f\). It can be shown that the relation (7) is exact within RPA \[55\]. Deviations can thus only arise for moderately or strongly coupled plasmas.

The range of applicability of formula (7) is investigated in Fig. 8 by comparison with full multi-component calculations. Both calculations were done using the HNC scheme for ions that interact via statically screened Coulomb forces (screening is determined by the electron

**Figure 5.** Ion-ion pair distribution in solid-density beryllium with \(T = 12\) eV. Shown are results from DFT-MD and multi-component HNC calculations using the KK-potential for the electron-ion interaction.

**Figure 6.** Comparison of the ionic structure factor from DFT-MD and multi-component HNC for beryllium as in Fig. 5. Note that the small \(k\)-behavior reflects differences for large distances in real space.
Figure 7. Comparison of HNC and DFT-MD results of the ion-ion structure for beryllium with the same parameters as in Fig. 5. The HNC calculations consider the ions only and use a screened Coulomb potential plus a strong short range repulsion as an effective interaction.

Figure 8. Partial structure factors of a CH plasma with different coupling strength which were calculated with the full two-component HNC approach or from HNC structure factors for one component plasmas via formula (7). The upper panels show data for a mass density of $\rho = 4.96 \text{gcm}^{-3}$ and a temperature of $T = 10 \text{eV}$ (left panel) and $T = 1 \text{eV}$ (right). The charge states of the ions are assumed to be $Z_H = 1$ and $Z_C = 3$ which results in coupling parameters of $\Gamma = 1.9$ and $\Gamma = 19$, respectively. The lower left panel shows results for the conditions measured in shock-driven plastics as presented in Ref. [30].
properties as usual). Clearly, we have increasing deviations of the two approaches if the coupling strength is increased. This makes the application of the approximate formula in the WDM region highly questionable. The lower panel also displays a line labelled ‘MSA’ which uses the mean spherical approximation to calculate the one component structure factor. The differences to the HNC(1comp) data reflect the deviating predictions of MSA and HNC [48].

3.4. Ion Structure of Highly Excited Solids

The warm dense matter region not only covers strongly coupled fluids but its definition often also applies for solids close to melting. DFT-MD simulations can be used in this parameter region without problems (indeed, DFT-MD was invented for condensed matter) whereas the HNC scheme is restricted to fluids as it uses radial symmetric functions.

Figure 9 shows a snap shot for warm graphite at normal density. One can clearly observe that the graphite layers are still intact and that the electron configuration is also very close to cold graphite, i.e., we have a small ionization degree. More precise information can be obtained

![Figure 9. Snap shot from a DFT-MD simulation of carbon with normal density and \( T = 0.2 \text{ eV} \). The brown and red areas label iso-surfaces of the electron density related to the L and K shell electrons, respectively. The cyan spheres are the carbon nuclei.](image)

![Figure 10. Ionic pair distribution for graphite at normal density and for different temperatures. These data were extracted from DFT-MD simulations. The lines correspond to different temperatures where the ion-ion pair distribution \( g(r) \) is, of course, more strongly peaked at lower temperatures.](image)
from condensed quantities such as the pair distribution shown in Fig. 10. All lines show the known order in graphite where the strong first peak is associated with the nearest neighbors in the plane and the next to ions in the planes above/below. At these graphs one can study the temperature effects on the ion structure close to melting as the peaks reduce in height and broaden with increasing temperature. This signature can be used as temperature diagnostics and also indicates melting as the well-defined spacing between peaks becomes more evenly spaced in the fluid.

4. Application to X-Ray Scattering as Plasma Diagnostics

The diagnostics of WDM states by means of x-ray scattering is one of the main applications for the structure calculations in the previous section. As for weakly coupled plasmas, the intensity of the radiation scattered under the angle \( \theta \) is given by

\[
P_s(\theta, \omega) d\Omega d\omega = \frac{4\pi N}{\pi A} S_{ee}^{tot}(k, \omega) \left[ 1 + \cos^2 \theta \right] d\Omega d\omega ,
\]

where \( k = (4\pi E_0/\hbar c) \sin(\theta/2) \) and \( \omega = (E_0 - E)/\hbar \) are the photon’s changes in wave number and frequency, respectively. \( P_0 \) is the incident flux, \( r_0 \) is the classical electron radius, \( N \) the number of electrons in the scattering volume and \( A \) the area through which the flux goes. The last term is a geometrical factor that accounts for the fact that the incoming photons are unpolarized as in many laser-driven experiments. The many-body properties, that determine the scattering intensity, are contained in the total electron structure factor \( S_{ee}^{tot} \).

Although only the electrons contribute to light scattering, the electron structure factor \( S_{ee}^{tot} \) must be calculated for a fully correlated electron-ion systems as the ion configuration strongly influences the electron properties. Moreover, both bound and free electrons must be included as the x-ray energy can drive internal excitations as well as bound-free transitions. Bound electrons also dominate elastic scattering in many WDM experiments [56, 27, 57, 30]. According to Chihara [58, 59] the total electron structure factor for the partially ionized materials under consideration can be decomposed into

\[
S_{ee}^{tot}(k, \omega) = \left[ f(k) + q(k) \right]^2 S_{ii}(k, \omega) + Z f S_{ee}^{0}(k, \omega) + S_{bf}(k, \omega).
\]

Here, the first term considers the contribution of electrons moving with the ions, that is, \( f(k) \) is the atomic or ionic form factor and \( q(k) \) is the density of the screening cloud in Fourier space. For light elements, \( f(k) \) can be described by hydrogen-like wave functions using the nuclear charge as a fitting parameter [33, 60]. The standard approach for \( q(k) \) is to use it in linear response [31] which is supported by the fact that the ion structure is also described well in this approximation (see section 3). The dynamic ion-ion structure factor can often be used in its static form \( S_{ii}(k, \omega) = S_{ii}(k) \delta(\omega) \) as laser-based x-ray sources are spectrally too broad to resolve the ion dynamics. Due to spectral resolution of the spectrometers used, this elastic contribution appears as a wide peak around \( \omega = 0 \) (Rayleigh feature). However, future experiments applying x-ray lasers may resolve the dynamics of the ion response yielding enhanced information on strong coupling effects and the mutual interactions of electrons and ions [61].

The second term in Eq. (9) described the dynamic response of the free electrons, that is, it is just the dynamic structure factor of a free electron gas [12]. This can be mainly described within RPA; more advanced approximations include the effect of electron-ion collisions, e.g., via a Mermin ansatz [62]. However, the determination of the collision frequency in WDM is an issue that is not fully resolved yet (see, e.g., Refs. [63, 64, 65, 66] for recent developments). The last remaining term determining the total electron structure factor describes contributions of internal excitations of the target electrons. For light elements from hydrogen to beryllium, these are of minor importance.
Figure 11. Synthetic scattering spectrum for 2.96 keV x-rays that experience a momentum transfer of $k = 10^{10} \text{m}^{-1}$ when scattered on beryllium at solid density and $T = 12 \text{eV}$ [28]. The Rayleigh peak has been artificially broadened by a Gaussian to mimic the limited experimental detector response. The electron feature is calculated for three different values of the collision frequency (see text).

Figure 11 shows an artificial scattering spectrum for warm dense beryllium. The two distinct features are related to the first and second terms of Eq. (9). Such model spectra are then fit to the experimentally measured data by changing temperature, density ionization degree. The best fit is then considered to yield the conditions investigated. Experimental spectra are also blurred due to different $k$ values and the detector response. We considered this effects by using a Gaussian for the ion feature that has the same weight as the first term in Eq. (9).

To obtain the data shown, we kept the first term constant and calculated the electron response with different collision frequencies as this quantity is not well understood. We used collision frequencies in Born approximation as defined in Ref. [63] and also frequencies that were artificially reduced (narrowest peak) or enhanced (broadest peak) by a factor of two to demonstrate the effect of the uncertainty in calculated collision frequencies. RPA data are not shown as these will give a high, very narrow peak. Clearly, the broadening of the plasmon peak plays an important role when interpreting the data. Thus, x-ray scattering might be also used to investigate the damping mechanism in WDM.

As both dynamic contributions are either reasonably well described or negligible, the structural information contained in the first term of Eq. (9) constitutes the major theoretical challenge for the description of x-ray scattering in WDM. The previous sections have given a state of the art description for this quantity based on classical integral equation and quantum simulations as DFT-MD from simple metals such as beryllium to multi-component fluids as plastics and highly excited solids.

Acknowledgements

We thankfully acknowledge fruitful discussions with Dr. Gregori (Oxford), Dr. Glenzer (Livermore) and Prof. Kraeft (Rostock) as well as financial support from EPSRC.

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