Dispersion force for materials relevant for micro- and nanodevices fabrication

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Abstract
The dispersion (van der Waals and Casimir) force between two semi-spaces is calculated using Lifshitz theory for different materials relevant for micro- and nanodevices fabrication, namely, gold, silicon, gallium arsenide, diamond and two types of diamond-like carbon, silicon carbide, silicon nitride and silicon dioxide. The calculations were performed using recent experimental optical data available in the literature, usually ranging from the far infrared up to the extreme ultraviolet bands of the electromagnetic spectrum. The results are presented in the form of a correction factor to the Casimir force predicted between perfect conductors, for the separation between the semi-spaces varying from 1 nm up to 1 \( \mu \)m. The relative importance of the contributions to the dispersion force of the optical properties in different spectral ranges is analysed. The role of temperature in semiconductors and insulators is also addressed. The results are meant to be useful for the estimation of the impact of the Casimir and van der Waals forces on the operational parameters of micro- and nanodevices.

1. Introduction
In recent years, as the size of microelectromechanical systems (MEMS) decreased, the distance between moving parts decreased correspondingly entering in the range of hundreds or even tens of nanometres. At such separations, the relatively large moving parts of MEMS experience an attractive force due to quantum fluctuations of the electromagnetic vacuum that can be relevant for the determination of their operational parameters [1, 2]. Borrowing a terminology frequently used in the realm of quantum field theory this attractive force is commonly referred to as the Casimir force [3]. Entering the realm of nanoelectromechanical systems (NEMS), shorter separations between moving parts are found which lie in the range of a few nanometres. In such a case, it has become usual to consider the effects of the well-known van der Waals force [4]. However, since the work of Lifshitz [5] the van der Waals and Casimir forces can be treated in a unified form resulting from the electromagnetic quantum vacuum fluctuations existing between two separated dielectric bodies. The van der Waals (Casimir) force arises as a limiting case for short (large) separations between the bodies. Because in our analysis we are going to cover separations ranging from 1 nm up to 1 \( \mu \)m, we cover both limits. For that reason, and to avoid this sometimes confusing terminology, which includes the concept of the retarded van der Waals force, we refer to the force here analysed simply as the dispersion force, a unifying terminology also found in the literature.

The role that dispersion forces may play in the determination of the operational parameters of MEMS and NEMS has been analysed theoretically in several instances [2, 4, 6] and determined experimentally in, for example, [1, 7, 8]. Different methods and approximations were used in those analyses to determine the resulting dispersion force: pairwise summation of the interatomic Lennard-Jones potential [4], a rough distance independent correction factor to the Casimir force between perfectly conducting plates [6] or the Lifshitz theory using actual optical data [1, 2] for the determination of the force between silicon plates, or simple estimates based on the results for highly idealized cases [8]. In fact, because the dispersion forces are highly dependent on the geometry of the interacting bodies and on their frequency...
dependent dielectric properties [3, 9, 10] there is no simple method of calculation that applied to every situation will always give reliable results.

Nevertheless, for simple geometries, involving large surfaces with small deviations from the plane parallel geometry, a powerful, reliable and relatively simple approach is to take into account the dielectric properties of the interacting bodies through the Lifshitz theory for the pressure resulting between two semi-spaces and the geometry through the Derjaguin approximation [3, 9, 10] as explained in the next section. However, results based on Lifshitz theory [5] are available in the literature solely for three materials of relevance for micro- and nanofabrication: gold and aluminium, for distances varying from less than 1 nm up to 1 μm [11], and single crystal silicon, for distances varying from 1 nm up to 1 μm [2]. In this paper we expand this list including results for amorphous silicon, crystalline gallium arsenide, crystalline diamond, two types of diamond-like carbon (DLC), cubic silicon carbide, amorphous silicon nitride and amorphous silicon dioxide, in the range 1 nm–1 μm.

This paper is organized as follows. In section 2 we briefly summarize how Lifshitz theory is used in order to calculate the pressure between two dielectric semi-spaces, and how this result can be used to approximate the force between dielectric non-planar bodies. In section 3 the results for the different materials we analyse are presented. We conclude in section 4.

2. Lifshitz theory and Dejarguin approximation

According to Lifshitz theory the dispersion force between two semi-spaces made of the same material and separated by a vacuum is a function of the frequency dependent complex dielectric function of the material, $\epsilon(\omega)$. The resulting pressure at a separation $d$ and at temperature $T$ can be written as [5]

$$ p^T(d) = -\frac{k_B T}{\pi^2 c^2} \times \sum_{l=0}^{\infty} \frac{\xi_l^3}{K} \int_1^\infty p^2 dp \left\{ \left[ \frac{K + \epsilon(\xi)^2 p}{K - \epsilon(\xi)^2 p} \right]^2 e^{2\xi dp} - 1 \right\}^{-1} + \left[ \frac{K + p}{K - p} \right]^2 e^{2\xi dp} - 1 \right\}^{-1}, $$

(1)

where $k_B$ denotes the Boltzmann constant, $c$ the speed of light, $K = K(i \xi) = \sqrt{p^2 - 1 + \epsilon(\xi)^2}$, $\xi_l = 2\pi k_B T / \hbar$ and the prime near the summation sign means that the zeroth term is taken with the coefficient 1/2. The sum in equation (1) converges rapidly for temperatures above a few tens of Kelvin; however, for lower temperatures the number of terms to be summed become too large and the use of the zero temperature approximation becomes computationally more appealing. When $k_B T \ll \hbar c / d$ we can replace the sum by an integral and the pressure becomes

$$ p^I(d) = -\frac{\hbar}{2\pi^2 c^2} \times \int_1^\infty p^2 dp \times \int_0^\infty \xi^3 d\xi \left\{ \left[ \frac{K + \epsilon(\xi)^2 p}{K - \epsilon(\xi)^2 p} \right]^2 e^{2\xi dp} - 1 \right\}^{-1} + \left[ \frac{K + p}{K - p} \right]^2 e^{2\xi dp} - 1 \right\}^{-1}. $$

(2)

At zero temperature and in the limit of perfectly conducting plates ($\epsilon \to \infty$) equation (2) recovers the now classical result for the Casimir force acting between parallel plates:

$$ p^{Cas}(d) = -\frac{\pi^2 \hbar c}{240 \pi^4 d^4}, $$

(3)

while for dielectrics separated by short distances the pressure results to be

$$ p^{anW}(d) = -\frac{A_H}{6\pi d^3}, $$

(4)

therefore recovering the van der Waals force ($A_H$ denotes the Hamaker constant).

Equations (1) and (2) depend on actual optical data through the complex dielectric function $\epsilon(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega)$. More specifically, we calculate the dielectric permittivity along the imaginary axes appearing in both equations, $\epsilon(i \xi)$, from $\epsilon(\omega)$ with the help of a Kramers–Kronig relation:

$$ \epsilon(i \xi) = 1 + \frac{2}{\pi} \int_0^\infty \frac{\epsilon_2(\omega)}{\omega (1 + \xi^2 / \omega^2)} d\omega. $$

(5)

In order to accurately calculate the pressure over a wide range of the separation $d$, the knowledge of $\epsilon_2(\omega)$ in a correspondingly wide range of frequencies is necessary, in such a way that the result of the approximate numerical integration performed to obtain $\epsilon(i \xi)$ is as close as possible to the exact result. In order to fulfil this requirement we considered the optical properties of the different materials in a range of frequencies ranging from infrared (IR) up to extreme ultraviolet (EUV) or x-ray. For all materials we consider, there are data available covering the interband transition region, in the visible and ultraviolet (UV) regions of the electromagnetic spectrum. This is the spectral region that gives the most important contribution to the dispersion force in the dielectric materials we consider. However, for large separations the contributions from IR region have to be considered while at the shortest distances that we consider contributions from EUV have to be taken into account, as is going to be evidenced by our analysis.

For some materials that we analyse, there are tabulated optical data covering the entire relevant spectral region, which can be interpolated and numerically integrated. However, for silicon nitride and silicon dioxide we have to perform an approximation resorting to the Ninham–Parsegian representation [9] of $\epsilon(i \xi)$ in the IR region. In this
representation $\epsilon(i\xi)$ is calculated based solely on the absorption strength ($C_i$) and relaxation frequency ($\omega_i$) of the most relevant absorption peaks (in any spectral region, in principle),

$$\epsilon(i\xi) = 1 + \sum_{i=1}^{N} \frac{C_i}{1 + (\xi/\omega_i)^2},$$

with the second term approximating the integral in equation (5). Therefore, in calculating $\epsilon(i\xi)$ for silicon nitride and silicon dioxide we add the contribution of each absorption peak in the IR region.

For gallium arsenide, silicon carbide, silicon nitride, and DLC, the optical data are limited to relatively low energies situated in the UV region of the spectrum. Intending to improve the results for the shortest distances that we consider we extend the data set by inclusion of the data on the index of refraction $n$ and extinction coefficient $k$ provided by the Center of X-Ray Optics at the Lawrence Berkeley National Laboratory [12]. These data result from the compilation of both experimental and theoretical data for elements with $Z = 1–92$ on the atomic scattering factors [13]. The resulting $n$ and $k$ (we remind the reader that $\epsilon_2 = 2nk$) are expected to be reliable for energies above a few tens of electronvolts since at such energies the effects of atomic bounds in the solid state system, not taken into account by the atomic scattering factors, become sufficiently small. We checked this expectation by a comparison with experimental data for $n$ and $k$ for several solids. The disagreement varied from less than 5% for crystalline silicon to more than 30% for germanium; however, on average the agreement was within 20% for energies above a few tens of electronvolts. We comment on the consequences of using such x-ray data in section 4.

The results for the pressure between semi-infinite parallel planes can be used for the approximate calculation of the pressure between surfaces of different geometries. Whenever the relative inclination or the curvature of the surfaces is sufficiently small and the geometries are sufficiently simple the Derjaguin approximation can be used [9, 10]. This approximation permits the results presented in the next section to be used for the calculation of the dispersion forces for a large class of MEMS and NEMS made from moving parts other than parallel plates.

3. Results

In this section we present the results for the dispersion force. However, instead of the resulting pressure we present the finite conductivity correction factor, $\eta(d)$ which is a measure of the influence of the finite conductivity on the Casimir force. This factor is defined as the ratio between the pressure given by Lifshitz theory and the Casimir pressure between perfect conductors, equation (3). It evidences more clearly the effects of the different optical properties for the different materials that we analyse. The actual pressure due to the dispersion force is therefore given by $p(d) = \eta(d)p^0(d)$. For instance, for a separation $d = 10$ nm the Casimir pressure predicted by equation (3) is $\sim 1$ atm, while the actual dispersion force is reduced by almost an order of magnitude.

For most materials we present $\eta(d)$ for different temperatures: 0, 300 and 700 K. The chosen temperatures are representative of cryogenic temperatures, ambient temperature and the high temperatures that may be found inside integrated circuits, respectively. When only one temperature is considered we take $T = 0$ K. Our results span the separation range 1 nm–1 $\mu$m. We do not consider larger distances because the dispersion forces become too small to be relevant in any practical MEMS or NEMS. On the other hand, the smallest separations we consider are already found in sophisticated NEMS such as the nanoresonator presented in [14], where a gap of only 20 nm exists between the moving parts.

Besides the curve for $\eta(d)$, for the most relevant cases we also provide a least-squares polynomial fit to the data points that can be readily used. The fitting polynomial is of the form $\eta(x) = a_0 + \sum_{n=1}^{5} a_n x^n$, where a new variable is used instead of $d$, namely, $x = [\log_{10}(1/d)]^{-1}$. The fitting for all cases is accurate within $\sim 1\%$ for $d > 3$ nm, but presents larger discrepancies for shorter distances, in some cases exceeding 4% at 1 nm. The order of the polynomial is the smallest one required to keep the accuracy $\sim 1\%$ for $d > 3$ nm and varied from 6 to 7.

3.1. Metals (gold)

Metals are widely used as a structural material for the fabrication of microsensors and microactuators, especially in RF MEMS, and were used in NEMS, for instance, on top of nanoresonators as conductive layers to provide a means of both induction and detection of motion [15] or to produce nanocantilevers [16], among many other applications. Aluminium (Al) and gold (Au) are among the most widely used metals in micro- and nanodevices, while nickel (Ni), chromium (Cr), titanium (Ti) and some metallic alloys were also used.

Due to their high electrical conductivity, metals are the materials that best approximate the perfect conductor boundary condition leading to the highest observable forces. For this reason they were used in all the recent experiments intended to measure the Casimir force with the highest accuracy [3]. The Casimir force for Al and Au was already investigated theoretically using Lifshitz theory [11]. We present the results for gold (Au) as representative of the metals used for micro- and nanofabrication to allow an immediate comparison with the results for the semiconductors and insulators we consider in this work. Here we use the same data set and further procedures as those employed in [11] obtaining the same results. The Casimir force was calculated at $T = 0$ K using equation (2). We do not consider higher temperatures because of the present controversy on how to specify the dielectric function for metals at zero frequency [17]. However, for a good conductor it is expected that the correction due to the non-zero temperature approaches that for perfect conductors, especially at large distances [3], being only slightly greater. The temperature corrected pressure between perfect conductors reads, to leading order in $T$,

$$p^T(d) = p^0(d) \left[ 1 + \frac{1}{3} \left( \frac{Td}{1145} \right) \right].$$

\[7\]
with the separation $d$ given in micrometres. According to this expression, at 300 K the force increases by just 0.15% at a separation of 1 $\mu$m. At 700 K, however, the correction is considerable at the same distance, the force increasing by 4.6%. But it decreases very rapidly and at $d = 500$ nm the correction is only 0.3%.

In figure 1 we present $\epsilon_2$ and $\eta$ for Au. We note that $\eta \sim 1$ at 1 $\mu$m and it decreases rapidly for shorter separations. Around 1 nm, $\eta$ changes linearly in the log-linear graph indicating that the force varies with $d^3$. This result is expected at short distances and characterizes the van der Waals force between two semi-spaces as seen from equation (4). The fitting function for gold at 0 K is $\eta(x) = 1.287 \times 10^{-5} - 5.810 \times 10^{-8}x + 1.088 \times 10^{-10}x^2 - 1.083 \times 10^{-12}x^3 + 6.035 \times 10^{-15}x^4 - 1.782 \times 10^{-18}x^5 + 2.178 \times 10^{-21}x^6$.

### 3.2. Silicon

Silicon in both its crystalline (c-Si) and polycrystalline forms is the most used material in MEMS and NEMS fabrication. Crystalline silicon is widely employed in processes involving bulk micromachining, while polysilicon in those where surface micromachining is required. Crystalline silicon is the best understood semiconductor, and its optical properties were thoroughly investigated. High quality optical data are available from the far infrared up to x-ray energies. Here we use the tabulated data of [18] for $\epsilon_2$ for energies ranging from 0.85 up to 3750 eV. In the IR region the interaction of light with the phonons is rather weak because silicon is a homopolar crystal and there are no active optical phonons. For this reason $\epsilon_2$ below 0.85 eV can be neglected [18].

As for any polycrystalline material, the precise optical properties of polysilicon are highly dependent on the sample properties; different deposition methods and post deposition treatments result in different optical properties [19], and the optical constants for different samples are available only for the visible spectral region. However, the available data on $n$ and $k$ indicate that the optical properties of any polysilicon sample are going to be between those of c-Si and that for amorphous silicon (a-Si) [19]. Therefore, the curves for $\epsilon_2$ and $\eta$ for c-Si and a-Si are the two limiting cases for polysilicon. For that reason and due to the fact that the optical data for a-Si are available in a wide energy range, we are going to present $\eta$ for a-Si instead of specific polysilicon samples. We use the tabulated data for a-Si of [18] ranging from 0.7 up to 48 eV.

The contributions from the IR region can be safely neglected as for c-Si and we do not extend $\epsilon_2$ for a-Si into the EUV region because our main interest is simply to have a reasonable bound for $\eta$. As discussed further in section 4 the lack of optical data beyond a few tens of electronvolts does not significantly affect the results for silicon for separations larger than a few nanometres.

In figure 2 we present $\epsilon_2$ and $\eta(d)$ for c-Si and a-Si. At $T = 0$ K, $\eta$ for a-Si is greater than that for c-Si for all $d$, and we expected that $\eta$ for polysilicon samples will be somewhere
between the two curves. The effect of the temperature is rather small for c-Si up to \( d \sim 300 \text{ nm} \) and becomes significant for larger separations only at \( T = 700 \text{ K} \). For a-Si, a similar dependence on \( T \) was observed. The fitting function for c-Si at 0 K is \( \eta(x) = -1.72448394 \times 10^3 + 7.63983980 \times 10^3 x - 1.40017845 \times 10^3 x^2 + 1.35873375 \times 10^3 x^3 - 7.36382628 \times 10^3 x^4 + 2.11392547 \times 10^3 x^5 - 2.51213744 \times 10^3 x^6 \) and for a-Si \( \eta(x) = -1.76475428 \times 10^3 + 7.81534655 \times 10^3 x - 1.43181362 \times 10^3 x^2 + 1.38892511 \times 10^3 x^3 - 7.52481833 \times 10^3 x^4 + 2.15945166 \times 10^3 x^5 - 2.56554021 \times 10^3 x^6 \).

### 3.3. Gallium arsenide

Gallium arsenide (GaAs) has been widely used in the production of MEMS and NEMS despite its, in many aspects, unattractive mechanical properties due to its compensating attractive electrical and optical properties, availability as commercial high quality single crystal wafers and the relatively easy control of deposition and bulk micromachining, among other reasons [20]. Only crystalline GaAs (c-GaAs) has been used in MEMS and NEMS fabrication and its amorphous form is rarely cited as a potentially useful material. For these reasons and due to the lack of optical data for amorphous GaAs [18] we analyse in this section solely the dispersion force for c-GaAs.

Because c-GaAs has two different atoms per unit cell and has ionic bonds, it has active optical phonons in the IR region. Therefore, in contrast to silicon, we cannot simply disregard the optical properties in the IR region and we resort to the tabulated optical data collected in [18] which spans the energy range from 0.01 up to 15 eV, which contains one IR resonance peak. Above 15 eV, the data presented in [18] are only for the extinction coefficient and do not include the index of refraction. However, experimental data on \( n \) and \( k \) above 9.5 eV are also available in [21]. A comparison between these data and that collected in [18] evidences considerable disagreement in the overlapping energy range corresponding to values of \( \epsilon_2 \) differing by more than 30%. The differences extend over larger energies when we compare solely \( k \) from both references. Due to this incompatibility we resort to the x-ray data to obtain approximate results for \( \epsilon_2 \) in the entire energy range above 15 eV. The x-ray data are available above 30 eV and \( \epsilon_2 \) for the region between 15 eV and this energy was obtained by a third order interpolation including points below 15 eV and above 30 eV. We expect the error due to the use of interpolated data to be acceptably small since a relatively smooth variation of \( \epsilon_2 \) in this region can be expected based on the data from [21].

In figure 3 we present \( \epsilon_2 \) and \( \eta(d) \) for c-GaAs. We note how \( \eta \) for c-Si and c-GaAs are quite similar with differences that rarely exceed 5%. The impact of the IR activity of GaAs on the dispersion force is rather small even for the largest distances we consider, leading to a dependence of \( \eta \) on the temperature that is similar to that for silicon. For c-GaAs at 0 K the fitting function is \( \eta(x) = -1.45232063 \times 10^3 + 6.45763597 \times 10^3 x - 1.18680052 \times 10^3 x^2 + 1.15456553 \times 10^3 x^3 - 6.27138396 \times 10^3 x^4 + 1.80393078 \times 10^3 x^5 - 2.14758254 \times 10^3 x^6 \).

### 3.4. Diamond and DLC

Diamond has been used in the fabrication of MEMS and NEMS in both its polycrystalline and amorphous forms (DLC). It is suited for devices operating in harsh environments due to its chemical inertness and high hardness [20] and for the fabrication of high frequency micro and nanomechanical resonators due to its large Young modulus, of the order of 1000 GPa, and relatively low density \( (\rho \sim 3.5 \text{ g cm}^{-3}) \).

Because the optical properties of polycrystalline diamond are highly sample dependent and the optical data are restricted to small spectral ranges, as for polysilicon, we do not present an analysis for this form of diamond. Instead we consider crystalline diamond (c-diamond), whose optical properties were measured from far infrared up to x-ray energies, and that can serve as a reference material. We use the tabulated data for crystalline diamond of [18] ranging from 5.5 eV up to 800 eV. \( \epsilon_2 \) below 5.5 eV can be safely neglected because diamond is highly transparent in the optical region and as for silicon the contributions from the IR region are small due to the absence of active optical phonons.

DLC is a metastable form of amorphous carbon containing a significant fraction of \( \text{sp}^3 \) bonds [22]. This terminology encompasses several forms of amorphous carbon including purely amorphous carbon (a-C) and its hydrogenated alloys (a-C:H) and the \( \text{sp}^3 \) bonding rich tetrahedral amorphous carbon (ta-C) and its hydrogenated alloys (ta-C:H) [22]. a-C and a-C:H have been widely used as protective coating for the disk and read/write head in magnetic hard disks and...
are currently being investigated as potential materials for MEMS fabrication having its low temperature deposition as an important advantage over materials such as SiC, polycrystalline and ultrananocrystalline diamond and ta-C [22,23]. Compared with other forms of DLC, ta-C is the one that best preserves the best qualities of diamond, possessing high mechanical hardness and chemical inertness. Due to these qualities ta-C is an extremely interesting prospective material for MEMS due to its superior wear-resistant qualities, resistance to stiction (i.e. a combination of stickiness and friction) and potential as a biocompatible material that could be used inside the human body for medical purposes without generating an allergic reaction [24].

The optical properties of the DLC can vary widely depending on the fraction of sp3 bonds and the hydrogen content. We consider two representative DLC samples, one for ta-C with a large sp3 content of 80% and another for a-C:H with a relatively low hydrogen concentration of 25%. The optical data for \( \varepsilon_2 \) for the ta-C sample were extracted from [25] for the energy range 1.7–40 eV. For energies above 40 eV we used x-ray data calculated considering a sample made from pure carbon and having the same density as measured in [25] \( \rho = 3.0 \text{ g cm}^{-3} \). Because there is a mismatch between the experimental and x-ray data in the range 30–40 eV of the order of 15% we actually use the x-ray data for energies above 50 eV softening the mismatch over the 10 eV gap between 40 and 50 eV using numerical interpolation. The optical data for a-C:H were extracted from [26] and spanned the energy range between 0.7 and 30 eV. As for ta-C we observed a considerable mismatch at 30 eV between experimental and x-ray data (the x-ray data were calculated for a sample having four carbon atoms for one hydrogen and the density obtained experimentally of \( \rho = 1.75 \text{ g cm}^{-3} \)) and used a 10 eV gap in order to soften the mismatch. Therefore, x-ray data were used above 40 eV. With regard to the IR activity of ta-C and a-C:H, it was experimentally verified [27] that both forms of DLC have low absorption in the IR region, and therefore \( \varepsilon_2 \) in the IR can be neglected.

In figure 4 we present \( \varepsilon_2 \) and \( \eta(d) \) for c-diamond and the two forms of DLC. The resulting correction factors \( \eta \) present interesting behaviour. At short distances, below approximately 100 nm the Casimir force for c-diamond is slightly larger than that for ta-C; however, for separations above 100 nm an inversion occurs. This inversion can be easily understood. The force at short distances is influenced mostly by the strength of the resonances in the UV region which are clearly weaker for ta-C as compared with c-diamond. At larger distances the force is influenced by lower frequency modes for which \( \varepsilon_2 \) is larger in the case of ta-C. It is interesting to also note the decrease in the dispersion force for a-C:H relative to c-diamond and ta-C, making a-C:H an interesting choice to minimize the Casimir force.

The fitting function for c-diamond at 0 K is the 7th order polynomial \( \eta(x) = -6.885 \times 10^{-6} + 3.537 \times 10^{3} x + 7.746 \times 10^{3} x^2 + 9.373 \times 10^{3} x^3 - 6.770 \times 10^{3} x^4 + 2.919 \times 10^{4} x^5 - 6.961 \times 10^{4} x^6 + 7.082 \times 10^{4} x^7 \).
3.6. Silicon nitride

Silicon nitride (SiN) is widely used in MEMS for electrical isolation, surface passivation, etch masking and as a mechanical material [20], being in the last case also used in NEMS, for instance, in the fabrication of nanoelectromechanical oscillators [30]. Silicon nitride is usually employed in its amorphous form and frequently it is also non-stoichiometric and may contain significant concentrations of hydrogen. Good optical data are available in a wide energy range for the amorphous stoichiometric silicon nitride (a-Si$_3$N$_4$) [31] and for crystalline stoichiometric β-Si$_3$N$_4$ [32]. Here we focus on the results for a-Si$_3$N$_4$ because SiN is usually employed in its amorphous form in MEMS and NEMS.

For a-Si$_3$N$_4$ we use the data from [31] which span the energy range 4–24 eV. There are two resonances in the IR region whose effects we introduce using equation (6) with $C_1 = 1.08$ and $\omega_1 = 0.9 \times 10^{14}$ rad s$^{-1}$, and $C_2 = 2.37$ and $\omega_2 = 1.64 \times 10^{14}$ rad s$^{-1}$ [33]. For energies above 30 eV we use x-ray data calculated for stoichiometric Si$_3$N$_4$ with density $\rho = 3.2$ g cm$^{-3}$ and use cubic interpolation between 24 and 30 eV. We note that the $\varepsilon_2$ generated using x-ray data is in very good agreement with the experimental data for β-Si$_3$N$_4$.

In figure 6 we present $\varepsilon_2$ and $\eta(d)$ for a-Si$_3$N$_4$. From the results for $\eta$ it can be concluded that the resulting Casimir force is smaller than that for the previously analysed materials. The influence of the IR activity is also noticeable, as for SiC, having a larger relative importance on $\eta$, that corresponds to a 34% increase in the force at 1 µm and 0 K. The effect of temperature is also large for a-Si$_3$N$_4$, leading to a 33% increase in the force at 1 µm and 700 K as compared with 0 K.

The fitting function for a-Si$_3$N$_4$ at 0 K is a 7th order polynomial, namely, $\eta(x) = -4.579 \times 10^{47} + 2.334 \times 10^{46} x - 5.071 \times 10^{45} x^2 + 6.088 \times 10^{44} x^3 - 4.362 \times 10^{43} x^4 + 1.866 \times 10^{42} x^5 - 4.134 \times 10^{41} x^6 + 4.453 \times 10^{40} x^7$.

3.7. Silicon dioxide

Silicon dioxide, in its amorphous form (a-SiO$_2$), is usually known for its applications in microelectronics as an electric insulator. More recently it has been widely used in the fabrication of MEMS and NEMS as a sacrificial layer material and has also found application as a structural material, for instance, for the fabrication of large suspended membranes and grating light valves [34]. Quartz, the crystalline form of SiO$_2$, has also been used as a structural material for the fabrication of MEMS, specially in microfluidics.

For both a-SiO$_2$ and quartz there are good optical data available in a wide range of energies and we resort to the most recent works. In [35] the data cover the range 1.5–42 eV for both forms of SiO$_2$, while in [36] the energy range 65–3000 eV is covered for the amorphous form. Due to the availability of recent data in a wider range for a-SiO$_2$ and its almost omnipresence in MEMS and NEMS we analyse the Casimir force for this form of silicon dioxide. However, due to the similarity between the optical properties of crystalline and

use the data on $\varepsilon_2$ of [29]. Above 30 eV we resort to x-ray data and use an interpolating function in the 20–30 eV range.

In figure 5 we present $\varepsilon_2$ and $\eta(d)$ for 3C–SiC. In order to determine the impact of the IR activity of the SiC on $\eta(d)$ we present in figure 5 $\eta$ calculated at 0 K without the contributions from the IR region (indicated by the label ‘No IR’ in the figure). The result is considerably smaller than that for the full spectrum at 0 K for distances above approximately 100 nm, demonstrating the importance of the IR activity for this material. More specifically, the relative increase due to the IR activity on the force is about 21% at a separation of 1 µm. For non-zero temperature we observe a larger relative increase in $\eta$ as compared with the materials analysed previously, specially for distances near 1 µm where it increases by 25% at 700 K compared with 0 K. This larger increase can be attributed to the contribution of the IR region. The different consequences on $\eta$ of the IR activity for GaAs and SiC can be attributed to the much stronger IR resonance peak of the later (by about a factor of 6) and to its occurrence at a higher energy around 0.1 eV, compared with 0.033 eV for GaAs.

As for c-diamond the fitting function for 3C–SiC at 0 K is a 7th order polynomial, namely, $\eta(x) = -4.674 \times 10^{5} + 2.362 \times 10^{4} x - 5.088 \times 10^{3} x^2 + 6.054 \times 10^{2} x^3 - 4.298 \times 10 x^4 + 1.821 \times 10 x^5 - 4.267 \times 10 x^6 + 4.264 \times 10 x^7$. 

![Figure 5](image-url) 

**Figure 5.** Upper panel: $\varepsilon_2$ as a function of photon energy. Lower panel: $\eta$ as a function of the separation distance $d$. Results are for silicon carbide.
amorphous SiO$_2$ evidenced in [35], our results are expected to be approximately valid for quartz.

Complementing the experimental data from [35, 36] we use x-ray data between 42 and 65 eV, which has shown very good agreement with both data sets between 30 eV and approximately 100 eV where data superposition exists. From the IR region we considered the existence of three resonances whose effects we introduce using equation (6) with $C_1 = 0.829$ and $\omega_1 = 0.867 \times 10^{14}$ rad s$^{-1}$, $C_2 = 0.095$ and $\omega_2 = 1.508 \times 10^{14}$ rad s$^{-1}$ and $C_3 = 0.798$ and $\omega_3 = 2.026 \times 10^{14}$ rad s$^{-1}$ [33].

In figure 7 we present $\varepsilon_2$ and $\eta(d)$ for a-SiO$_2$. From the results for $\eta$ it can be concluded that the resulting dispersion force is considerably smaller than that for the previously analysed materials, a result attributable to the largest band gap of about 8.3 eV [37]. The influence of the IR activity is also the strongest amongst all the materials we analysed increasing the force by 74% at 1 $\mu$m and 0 K. The effect of temperature is also rather large, leading to a 52% increase on the force at 1 $\mu$m and 700 K as compared with 0 K.

The fitting function for SiO$_2$ at 0 K is a 7th order polynomial, namely, $\eta(x) = -1.840 \times 10^{3} + 9.416 \times 10^{2} x - 2.053 \times 10^{1} x^2 + 2.475 \times 10^{1} x^3 - 1.780 \times 10^{0} x^4 + 7.646 \times 10^{0} x^5 - 1.815 \times 10^{0} x^6 + 1.838 \times 10^{0} x^7$. 

3.8. Mixed materials

As our last result, we present $\eta$ for combinations of different materials in each of the two semi-spaces. Each semi-space, in practice, corresponds to each of the two parts of a given MEMS separated by an air gap (approximated here by a vacuum with no loss of rigour) and close enough to interact through the dispersion force. Each semi-space is filled with only one material at a time, but now one semi-space contains one material and the other semi-space a different material. For this case we use a generalization of equation (2) for the pressure between semi-spaces made from different materials found, for instance, in [38]. As representative of all possible combinations we consider the following three combinations of Au, c-Si and a-SiO$_2$: Au–Si, Au–SiO$_2$ and Si–SiO$_2$. They represent the three possible combinations conductor–semiconductor, conductor–insulator and semiconductor–insulator. The results for $\eta$ are presented in figure 8, where, as a reference, we also reproduce the results for Au, Si and SiO$_2$. It can be seen that, as could be expected, the resulting force is always between that produced for each material separately.

4. Discussions and conclusion

In performing our calculations we used the most recent and complete optical data available for each material in order to derive the most accurate results. However, even the
best tabulated optical data rely on results from different experiments based on different samples and methodologies covering different, and in many cases, not overlapping spectral regions that must be interpolated or modelled theoretically [18, 31]. Besides there may exist a significant disagreement between experiments, of the order of tens of per cent, as pointed out in section 3.3 for GaAs and as verified by the authors also for the case of 3C–SiC and a-SiO2 when the results from [18] and [29] and [35] and [39] were compared, respectively. Therefore, an analysis of the expected uncertainties in our theoretical predictions is necessary.

The result for gold must be considered taking into account the thorough analysis performed in [40] that has shown that large uncertainties, around 5%, must be assumed for the predicted force between gold plates. However, the analysis performed for gold cannot be extended for semiconductors and insulators. We can assume conservatively that δη of a-SiO2, the effects of the temperature are already noticeable at 700 K for silicon, gallium arsenide and diamond the effect is 5% be assumed. In the case of Au, c-Si and a-SiO2.

Table 1. Maximum uncertainty in η due to variations on ε2. Approximate values for small and large separation d.}

| Material (δε2) | δη (small d) | δη (large d) |
|--------------|--------------|--------------|
| c-S (2%)     | 1.6%         | 0.9%         |
| c-GaAs (2%)  | 1.7%         | 0.9%         |
| c-diamond (2%) | 2.0%   | 1.4%         |
| 3C–SiC (5%)  | 5.3%         | 3.2%         |
| a-Si3N4 (5%) | 5.8%         | 3.6%         |
| a-SiO2 (2%)  | 2.9%         | 2.0%         |

Figure 8. η as a function of the separation distance d. Results are for two different materials on each semi-space. The continuous lines are (from the top down) for Au, c-Si and a-SiO2.

For larger distances δη decreases to approximately 70% of δε2 for both materials. As a reference we present in table 1 the maximum and minimum δη as a function of δε2 for the most relevant semiconductors and insulators we considered. The general trend for the uncertainty is that it decreases rapidly from its maximum at 1 nm to a value close to its minimum for d ∼ 100 nm and is almost a constant for larger d reaching a minimum at 1 µm.

For c-GaAs, 3C–SiC, a-Si3N4 and DLC another source of uncertainty results from the use of x-ray data. As already mentioned in section 2 a comparison between the experimental and x-ray data for several materials, such as aluminium, copper, silicon and germanium, evidences that the x-ray data are precise within about 20% for energies above 30 eV. The actual disagreement could be smaller, since the x-ray data tend to agree well (within 10%) with the most recent, and presumably more precise, experimental data for materials such as silicon and silicon dioxide. We can assume conservatively that δε2 for such energies is about 20%. In order to estimate how this uncertainty affects η, we first note that for the semiconductors and insulators that we are considering δε2 above 30 eV amounts to at most 6% of η for d ∼ 1 nm, 3% at d ∼ 10 nm and contributes less than 1.5% at 100 nm. Therefore, the extra uncertainty due to the x-ray data is at most approximately 1.2% at 1 nm, 0.6% at 10 nm and 0.3% at 100 nm and can be neglected for larger separations. It is to be noted that this extra uncertainty results in an error that is much smaller than the error resulting from the neglect of ε2 above 30 eV, therefore justifying the use of the x-ray data when no experimental data are available.

The above uncertainty analysis demonstrates that a complex relationship exists between the uncertainty in the optical data and the theoretical prediction of the Casimir force. Therefore, for precise experiments a careful analysis must be performed for each material and experimental condition. However, the results we present are useful for theoretical estimates of the impact of the dispersion force on the operational parameters of MEMS and NEMS.

We also addressed the role of temperature in the expected dispersion force since MEMS and NEMS operating in real conditions may be subject to high temperatures that alter the force. For all materials but SiO2 the effect of the ambient temperature of T = 300 K on the force is rather small. At T = 700 K for silicon, gallium arsenide and diamond the effect of temperature is not so severe but exceeds the approximate result for metals by at least a factor of 2 for d ∼ 1 µm. However, for materials with strong IR activity, SiC, Si3N4 and SiO2, the effects of the temperature are already noticeable at
shorter distances for $T = 700 \text{ K}$ and are rather large for $d$ in the range of hundreds of nanometres. At this point, it is worth mentioning that no experiment performed to date has measured the dependence of the dispersion force on temperature but, according to our results, materials with strong IR activity are the most adequate for such an experiment due to the greater sensitivity of the force to temperature.

Our analysis also evidences how significant can be the contribution for the dispersion force coming from the IR region through the results for SiC, Si$_3$N$_4$ and SiO$_2$. The effects of the IR activity are already noticeable at distances in the range of a few tens of nanometres and increase the dispersion force by tens of per cent at larger separations even at $0 \text{ K}$. Therefore, due to its potential effects on the dispersion force, knowledge of the IR optical behaviour of a given material is mandatory when this force is to be calculated for distances ranging from tens up to hundreds of nanometres. The IR spectral region can be neglected only after a careful analysis.

When the dispersion forces are to be calculated for short distances, smaller than about 100 nm, knowledge of the optical properties in the UV region is required. We considered typically the optical properties up to a few hundreds of electronvolts, corresponding to the EUV spectral region. However, as expected for semiconductors and insulators, the more important contribution to the dispersion force over the entire interval considered for the separation $d$ comes from the interband transition region, usually extending from $\sim 1 \text{ eV}$ up to $\sim 20 \text{ eV}$.

The results presented so far for the dispersion force can be used with no restrictions when the MEMS and NEMS surfaces are made of the materials we analysed. However, it is often true that those surfaces are contaminated by oxides, water and hydrocarbons, and for this reason we performed an analysis in order to estimate the effects of such contaminants. Since the dispersion force in current and near future MEMS and NEMS will more often be considered as a first order correction to the total force acting on the system, small corrections to that force can be seen as second order corrections which can usually be ignored. We analysed the extent to which the presence of contaminants can be considered as a second order correction to the total force.

The dispersion force between two semi-spaces made from the same material, both covered with a thin layer made from a second material, can be calculated using equation (4.24) presented in [3]. We use that equation with the thin layer representing the contaminant and consider the effect of only one contaminant at a time for representative material combinations. Let us first consider the effect of the ubiquitous oxide layer on top of silicon. The oxide layer in this case is usually a few nanometres thick [42]. Assuming, for the sake of simplicity, that the oxide layer is made entirely from SiO$_2$, the thickness, for instance, of a 2 nm thick oxide layer alters the dispersion force by more than 20% for a separation smaller than approximately 35 nm. The effect of the presence of the oxide layer is to decrease the force, as compared with the force produced between pure silicon slabs separated by the same distance. This result should be expected since the dispersion force between pure SiO$_2$ slabs is smaller than that for silicon. The effect of the SiO$_2$ layer is strongly dependent upon the layer thickness; it decreases very rapidly as the layer gets thinner but increases significantly for thicker layers. We also note that only for very small separations, below 2 nm, the presence of the oxide layer dominates the result for the dispersion force for 2 nm thick oxide layers.

In the case of contamination by water, it was verified that the thickness of the water layer on top of silicon never exceeds 0.5 nm [42]. The correction to the dispersion force due to a water layer on top of silicon, with this maximum thickness, is small and surpasses 20% only for separations below 10 nm. Such a water layer has a similar impact on the force, whether on top of gold or SiO$_2$. Finally, the presence of hydrocarbons on top of silicon, gold and SiO$_2$ is expected to have an impact on the dispersion force similar to that of water, due to their similar optical properties in the UV spectral region (see section 11.5 of [43]). We can summarize the results on the effects of contaminants by saying that their presence is of secondary importance usually down to separations of 50 nm.

We have just seen that the dispersion force depends on the thickness of the materials layers. However, it is beyond the scope of this work to consider further the effects of the layer thickness. We only mention that our results for the correction factor, derived using an expression that is exact only for two semi-spaces, can be used when the material layers are sufficiently thick to be approximated as two semi-spaces. For metals this corresponds to a thickness larger than a few tens of nanometres, while for semiconductors and insulators a thickness larger than a few hundreds of nanometres is required.

To conclude, we note that the dispersion forces for the different materials relevant for micro- and nanodevices fabrication can vary considerably. When large dispersion forces are desirable, good conductors or small band gap semiconductors should be used. However, in order to minimize the dispersion force, insulators are recommended. The results for diamond and DLC are an example of how the dispersion force can be tailored by chemical or physical changes of a given material as a strategy to control the dispersion forces in MEMS and NEMS.

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References

[1] Chan H B, Aksyuk V A, Kleiman R N, Bishop D J and Capasso F 2001 Science 291 1941
[2] Gusso A and Delben G J 2006 Sensors Actuators A 135 792
[3] Bordag M, Mohideen U and Mostepanenko V M 2001 Phys. Rep. 353 1
[4] Dequesnes M, Rotkin S V and Aluru N R 2002 Nanotechnology 13 120
[5] Lifshitz E M 1956 Sov. Phys.–JETP 2 73
[6] Serry F M, Walliser D and Maclay G J 1995 J. Microelectromech. Syst. 4 193
[7] Ke C and Espinosa H D 2006 Small 12 1484
[8] Buks E and Roukes M L 2001 Europhys. Lett. 54 220
[9] Hunter R J 2001 Foundations of Colloid Science (Oxford: Oxford University Press)
[10] Butt H J, Graf K and Kappl M 2006 Physics and Chemistry of Interfaces (Weinheim: Wiley-VCH)
[11] Klimchitskaya G L, Mohideen U and Mostepanenko V M 1999 Phys. Rev. A 60 3487
[12] See the url http://henke.lbl.gov/optical_constants/
[13] Henke B L, Gullikson E M and Davis J C 1993 At. Data Nucl. Data Tables 54 181
[14] Agache V, Legrand B, Collard D, Buechaillet L and Fujita H 2005 Appl. Phys. Lett. 86 213104
[15] Ekinci K L and Roukes M L 2005 Rev. Sci. Instrum. 76 061101
[16] Davis Z J and Boisen A 2005 Proc. 5th IEEE Conf. on Nanotechnology (Nagoya, Japan)
[17] Mostepanenko V M, Bezerra V B, Decca R S, Geyer B, Fishbach E, Klimchitskaya G L, Krause D E, López D and Romero C 2006 J. Phys. A: Math. Gen. 39 6589
[18] Adachi S 1999 Optical Constants of Crystalline and Amorphous Semiconductors (Boston, MA: Kluwer)
[19] Modreanu M, Gartner M, Tomozeiu N, Cobianu C, Cospin P and Gavrila R 2001 Proc. Semiconductor Conf. (Sinaia) vol 2 (Piscataway, NJ: IEEE) p 387
[20] Bushan B (ed) 2004 Springer Handbook of Nanotechnology (Berlin: Springer)
[21] Windt D L 1991 Appl. Opt. 30 15
[22] Robertson J 2002 Mater. Sci. Eng. R 37 129
[23] Peiner E, Tibrewala A, Bandorf R, Lühthe H, Doering L and Limmer W 2007 J. Micromech. Microeng. 17 S83
[24] Extracted from http://www-g.eng.cam.ac.uk/edm/research/mems/SAW.html
[25] Waidmann S, Knüfer M, Fink J, Kleinsorge B and Robertson J 2001 J. Appl. Phys. 89 3783
[26] Fink J, Müller-Heinzlering Th, Pflüger J, Scheerer B, Dischler B, Koidl P, Bubenzer A and Sah R E 1984 Phys. Rev. B 30 4713
[27] Chen Z Y and Zao J P 2000 J. Appl. Phys. 87 4268
[28] Chou L H and Wang H W 1993 J. Appl. Phys. 74 4673
[29] Vendana M, Moliana P, Bastawrosa A and Anderegg J 2005 Mater. Sci. Semicond. Process. 8 630
[30] Carreno M N P and Lopes A T 2004 J. Non-Cryst. Solids 338 490
[31] Palik E D (ed) 1985 Handbook of Optical Constants of Solids (Orlando, FL: Academic)
[32] Müllerjeans H and French R H 2000 Microsc. Microanal. 6 297
[33] Trisman J I, Carlisle C B and Monteverde R 2004 Photonics West 2004—Machanisation and Microfabrication Symp. (San José, CA, USA)
[34] Tan G L, Lemon M F, Jones D J and French R H 2005 Phys. Rev. B 72 205117
[35] Filatova E, Lukyanov V, Barchewitz R, André J-M, Idir M and Stemmler Ph 1999 J. Phys.: Condens. Matter 11 3355
[36] Phillip H R 1966 Solid State Commun. 4 73
[37] Milonni P W 1993 The Quantum Vacuum: An Introduction to Quantum Electrodynamics (San Diego, CA: Academic)
[38] Bekhti W and Ghamnia M 2004 Catal. Today 89 303
[39] Pirozhenko I, Lambrecht A and Svetovoy V B 2006 New J. Phys. 8 238
[40] Aspnes D E and Studna A A 1983 Phys. Rev. B 27 985
[41] Kenny J M, Netterfield R P, Wielunski L S and Beaglehole D 1999 IEEE Trans. Instrum. Meas. 48 233
[42] Israelachvili J N 1998 Intermolecular and Surface Forces (San Diego, CA: Academic)