In the last few years, several experiments based on non-contact force microscopy (nc-AFM) have been performed that revealed a strong dependence on non-contact force in the tip-sample interaction [Volkodav07, Gussos08]. A particularly relevant result was that obtained by Gatzmann and Funck [Gatzmann01] for the dissipation between an aluminum coated silicon tip and a crystalline gold surface. They measured a significant dissipation that could be modeled as a viscous damping with a coefficient of friction varying as $d^2$, where $d$ denotes the tip-sample separation as measured from the contact. While this experimental result remains without satisfactory theoretical explanation, several physical models predict a non-contact friction that is a function of the tip-sample force [Volkodav07, Gussos11]. In order to discriminate the correct physical model from the experimental results for the dissipation an adequate modeling of the tip-sample force is required. So far, the long range component of the tip-sample force has been modeled simply by using the pressure predicted between two semi-infinite spaces by the well-known Lifshitz theory (Lifshitz76) in conjunction with proximity force approximation [Holmér92]. The resulting tip-sample force has the characteristics of $d^3$ dependence at short separations in the case of a spherical tip end. In order to improve the modeling of tip-sample force we include the effects of the dielectric function surface gradient and surface roughness.

Some aspects of the surface effects on the dielectric function close to the surface have recently been incorporated in the calculation of the Casimir force for the case of metals [Marusin11]. However, to the best of our knowledge, the dielectric function variation close to the surface of semiconductors and insulators has not yet been taken into account. While the changes in the electronic properties at the surface of dielectric materials has been extensively studied [Loh95], only recently the dielectric function was calculated as a function of the surface distance. Mendoza et al. [Mendoza06] calculated the linear susceptibility $\chi_0(\omega)$, which is related to the dielectric function by $\varepsilon(\omega) = 1 + 4\pi\chi_0(\omega)$, for crystalline silicon. The results for the surface part of the anisotropic susceptibility for hydrogen-terminated surfaces are reproduced in Fig. 1. These results suggest that, under the simplifying assumption $\kappa_{g,2}^{2}(\omega) = \kappa_{ss}^{2}(\omega) = \kappa_{s,1}^{2}(\omega) = \kappa_{s,ss}^{2}(\omega)$, the spatial variation in the $\varepsilon$ direction should be described by a sigmoid function

$$\varepsilon(\omega) = \varepsilon(\infty) + \frac{(\varepsilon_0 - \varepsilon(\infty))}{1 + (\omega_0^2/\omega^2)^2},$$

where $\varepsilon_0$ is the linear susceptibility at zero frequency, $\varepsilon(\omega)$ is the real part of the relative dielectric function at frequency $\omega$, $\omega_0$ is the characteristic frequency, and $\varepsilon(\infty)$ is the static dielectric constant.

For the purpose of calculating the influence of the surface dielectric function gradient on the Casimir force we have taken $\varepsilon(\omega)$ to vary as a quadratic function within a transition region of thickness $h$. The Casimir force is calculated using a multilayer approximation. Within the multilayer formalism developed by Tomas [Tomas02] and Riazi et al. [Riazi03] the pressure between two multilayer slabs is given by

$$P(z) = \frac{1}{3\pi^2} \int_{0}^{\infty} d\omega \int_{0}^{\infty} d\omega' \frac{\varepsilon(\omega)\varepsilon(\omega')}{\omega^2 + \omega'^2} P_{g,2}^{2}(\omega,\omega') z,$$

where $P_{g,2}^{2}(\omega,\omega')$ are the generalized Fresnel reflection coefficients for the $x$ and $y$ polarized waves reflecting from the stacks of layers above (subscript 1) and below (subscript 2) the gap. $P(z)$ is a Fourier transform of $P_{g,2}^{2}(\omega,\omega')$, i.e.,$P(z) = \int_{0}^{\infty} d\omega \int_{0}^{\infty} d\omega' P_{g,2}^{2}(\omega,\omega') e^{i\omega z}$. In Fig. 2a we present a set of predictions based on this analytical results derived by Parsegian and Weiss [Parsegian72] for the non-retarded Casimir force between two semi-infinite spaces covered with slabs of thickness $D$ having an exponentially varying dielectric function of the form $\varepsilon(z) = \epsilon(0)e^{a|z|}$ with $a > 0$ varying between that of vacuum and bulk crystalline silicon $\varepsilon(0)$, as a function of the separation for the pressure (1)

$$P(z) = \frac{1}{3\pi^2} \int_{0}^{\infty} d\omega \int_{0}^{\infty} d\omega' \frac{\varepsilon(\omega)\varepsilon(\omega')}{\omega^2 + \omega'^2} P_{g,2}^{2}(\omega,\omega') z,$$

where $J_1(\frac{\pi}{D}) = \frac{1}{\pi} [\sin(\pi D/\lambda) - \sin(\pi d/\lambda)]$ and $J_0(\pi d/\lambda)$. It can be seen in Fig. 2a) that the prediction based on the multilayer approach in the non-retarded regime, obtained by taking $D = 0$, coincides with the result obtained from Eq. (2) for the non-retarded Casimir force. For the sake of further comparison, the force for sharp boundaries is also shown in Fig. 3a) which results to be larger than that for the case with the dielectric function gradient. At this point, it is worth to note that a general consequence of the presence of surface layers having $\varepsilon^{2}(\omega)$ with values varying between those of the gap dielectric function and those of the bulk is not only to decrease the force compared to those for sharp boundaries, but also to change the dependence of the Casimir force on the gap $d$. Due to the relevance of a precise knowledge of the dependence of the Casimir force on the tip-sample separation for interpretation of nc-AFM measurements, we have also analyzed how the expected dependence of the force on the separation $d$ of the form $F(d) \sim d^{-p}$ changes as a function of the surface separation. For this purpose it is useful to calculate the effective, or local, exponent $p$ which is calculated as $p = \alpha \Gamma(1 + 1/\alpha)$ (3). The resulting exponent is presented in Fig. 2b). It can be seen that the exponent is able to fit qualitatively from the expected value of $p = 3/2$. The general trend is the exponent to decrease for shorter separations, indicating a slower rate of change of the force, the decrease being larger the thicker the region of the order of $10^{-4}$.

Figure 1 - a) Anisotropic susceptibility for hydrogen terminated silicon surfaces (Mendoza06) and b) static dielectric permittivity as computed for a hydrogen terminated silicon slab (Gatzmann01).

Figure 2 - a) Pressure between two crystalline silicon semi-spaces with sharp boundaries (red curves), and covered with a 1 nm thick layer with exponentially varying dielectric function (black function). Dashed curves represent analytical results with retardation disregarded, and the continuous curves the results using the full Lifshitz theory (red) and a multilayer approach with 3 layers (black). The circles are the results for the multilayer approach being limited by an infinity speed of light,

$\kappa_{g,2}^{2}(\omega) = \kappa_{s,1}^{2}(\omega) = \kappa_{s,ss}^{2}(\omega)$

These results suggest that, under the simplifying assumption $\kappa_{g,2}^{2}(\omega) = \kappa_{ss}^{2}(\omega) = \kappa_{s,1}^{2}(\omega) = \kappa_{s,ss}^{2}(\omega)$, the spatial variation in the $\varepsilon$ direction should be described by a sigmoid function

$$\varepsilon(\omega) = \varepsilon(\infty) + \frac{(\varepsilon_0 - \varepsilon(\infty))}{1 + (\omega_0^2/\omega^2)^2},$$

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Figure 3 - a) The ratio between the Casimir force with a dielectric function surface gradient $P_{g,2}^{2}(\omega) = \kappa_{ss}^{2}(\omega)$ (black) and the Casimir force $P_{g,2}^{2}(\omega) = \kappa_{ss}^{2}(\omega)$ (red). The curves are for $\omega = 0.5$ (blue), 0.69 (red). The red dashed line is the ratio for the tip-sample force $P_{g,2}^{2}(\omega) = 0.7$ (red). Effective exponent for the Casimir force between two silicon nanowires with sharp (black/dotted) and smooth (quadrant) boundaries (black/full) and for the tip-sample force with sharp (red/dotted) and smooth boundaries (red/full).