LAO/STO and oxygen vacancies: dielectric modeling

Sohrab Ismail-Beigi

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Let's model the LAO/STO system as two dielectrics films of infinite extent in the xy plane and finite slabs in the z direction. The dielectric constant of LAO will be ϵ_1 and that of STO will be ϵ_2. The thicknesses will be d_1 and d_2. The z axis runs orthogonal to these films: $z = 0$ will be the LAO surface, $z > 0$ will be the vacuum above the LAO film, $z = -d_1$ will be the LAO/STO interface, and $z = -d_1 - d_2$ will be the STO/vaccum interface. We will be doing classical dielectric modeling of this system.

We are interested in the fields created by oxygen vacancies on the LAO surface at $z = 0$ and the corresponding electrons that will end up at the LAO/STO interface at $z = -d_1$. These will be our free charges: at $z = 0$ we will have $\sigma_+(x, y)$ for the positive oxygen vacancy and at $z = -d_1$ we will have $\sigma_-(x, y)$ for the electron gas. The system is net neutral so the integral of σ_+ is opposite to that of σ_-. We are assuming these free charges are very narrow in the z direction. Also, we assume they have cylindrical symmetry about the z axis.

The electrostatic problem we want to solve is

$$\nabla \cdot (\epsilon(z)\nabla\phi) = -4\pi\rho_{free}$$

where

$$\epsilon(z) = \begin{cases} 1 & \text{for} \quad 0 < z \\ \epsilon_1 & \text{for} \quad -d_1 < z < 0 \\ \epsilon_2 & \text{for} \quad -d_1 - d_2 < z < -d_1 \\ 1 & \text{for} \quad z < -d_1 - d_2 \end{cases}$$

and

$$\rho_{free}(x, y, z) = \delta(z)\sigma_+(x, y) + \delta(z + d_1)\sigma_-(x, y)\,.$$

Away from the boundaries, we have usual Laplace equation. We will work in Fourier space in the xy plane but keep the real space z description. Thus the potential will be in mixed variables $\tilde{\phi}(k_x, k_y, z)$ and we will denote $k = (k_x, k_y)$. In these variables, $\tilde{\phi}$ is easy to find in regions where $\epsilon(z)$ is constant:

$$\tilde{\phi} = \alpha e^{kz} + \beta e^{-kz}$$

for constants α and β. Thus we now have a boundary problem of matching the value and derivatives of $\tilde{\phi}$ at the three boundaries at hand. Also, we assume the potential goes to zero for $z \to \pm\infty$.

Thus, we will therefore be seeking a solution of the form

$$\tilde{\phi}(k,z) = \begin{cases} Ae^{-kz} & \text{for} \quad 0 < z \\ A_1 e^{-kz} + B_1 e^{kz} & \text{for} \quad -d_1 < z < 0 \\ A_2 e^{-kz} + B_2 e^{kz} & \text{for} \quad -d_1 - d_2 < z < -d_1 \\ Be^{kz} & \text{for} \quad z < -d_1 - d_2 \end{cases} .$$

The continuity conditions are

$$A = A_1 + B_1 \quad , \quad A_1 + B_1 e^{-2kd_1} = A_2 + B_2 e^{-2kd_1} \quad , \quad A_1 + B_1 e^{-2k(d_1+d_2)} = Be^{-2k(d_1+d_2)}$$

while the derivative discontinuity conditions at some z come from the general relation

$$\epsilon(z^+)\frac{d\tilde{\phi}}{dz}\Big|_{z^+} - \epsilon(z^-)\frac{d\tilde{\phi}}{dz}\Big|_{z^-} = -4\pi\tilde{\sigma}(k,z)$$

so we have

$$\begin{aligned} A + \epsilon_1(B_1 - A_1) &= 4\pi\tilde{\sigma}_+/k \\ \epsilon_1(A_1 - B_1 e^{-2kd_1}) + \epsilon_2(B_2 e^{-2kd_1} - A_2) &= 4\pi\tilde{\sigma}_- e^{-kd_1}/k \\ \epsilon_2(A_2 - B_2 e^{-2k(d_1+d_2)}) + Be^{-2k(d_1+d_2)} &= 0\,. \end{aligned}$$

Plugging all into Mathematica and solving for the quantity of interest, A, gives the wonderful mess

$$A = \frac{4\pi}{k}\cdot\frac{\epsilon_2\tilde{\sigma}_+(1-u)(1+\epsilon_2-(\epsilon_2-1)v)+\epsilon_1(\tilde{\sigma}_+ + 2\tilde{\sigma}_-\sqrt{u}+\tilde{\sigma}_+ u)(1+\epsilon_2+(\epsilon_2-1)v)}{\epsilon_2(1-u)(1+\epsilon_2-(\epsilon_2-1)v)+\epsilon_1^2(1-u)(1+\epsilon_2+(\epsilon_2-1)v)+\epsilon_1(1+u)((1+\epsilon_2)^2-(\epsilon_2-1)^2 v)}$$

where we've shortened

$$u \equiv e^{-2kd_1} \quad , \quad v \equiv e^{-2kd_2}\,.$$

The long denominator of A goes to $8\epsilon_1\epsilon_2$ for $k=0$ and to $(\epsilon_1+1)(\epsilon_2+1)(\epsilon_1+\epsilon_2)$ for large k. The derivative of the denominator versus k at $k=0$ is $4(d_2\epsilon_1(\epsilon_2-1)^2 + d_1\epsilon_2(\epsilon_1-1)^2)$. For applicable conditions $1 \ll \epsilon_1 \approx 30 \ll \epsilon_2 \approx 300$, the value at $k=0$ is $8\epsilon_1\epsilon_2 \approx 7.2\times10^4$ and slope versus k is $\approx 4d_2\epsilon_1\epsilon_2^2 \approx d_2 \times 1.08\times10^7$ and its value at large k is $\approx \epsilon_1\epsilon_2^2 \approx 2.7\times10^6$.

We can also find the total charge density $\tilde{\Sigma}(k,z)$ on the various planes $z = 0, -d_1, -d_2$ by just computing the discontinuity in the electric field $-d\tilde{\phi}/dz$. We have

$$\begin{aligned} \tilde{\Sigma}_0(k) &= \tilde{\Sigma}(k, z=0) = \frac{k}{4\pi}\cdot(A + B_1 - A_1) \\ \tilde{\Sigma}_1(k) &= \tilde{\Sigma}(k, z=-d_1) = \frac{k}{4\pi}\cdot(A_1 e^{kd_1} - B_1 e^{-kd_1} + B_2 e^{-kd_1} - A_2 e^{kd_1}) \\ \tilde{\Sigma}_2(k) &= \tilde{\Sigma}(k, z=-d_1-d_2) = \frac{k}{4\pi}\cdot(A_2 e^{k(d_1+d_2)} - B_e^{-k(d_1+d_2)} + Be^{-k(d_1+d_2)}) \end{aligned}$$

A is of interest as it gives the potential of the system on the $z=0$ plane. So we will have

$$\phi(x,y,z=0) = \int \frac{dk_x dk_y}{(2\pi)^2} e^{ik_x x + ik_y y} A(k) = \int_0^\infty dk\,\frac{k}{2\pi}\,A(k)J_0(k\rho)$$

where $\rho = \sqrt{x^2+y^2}$ and we've assumed cylindrical symmetry. Here are some integrals for reference:

$$A(k) = \frac{2\pi}{k} \;\rightarrow\; \phi(\rho, z=0) = \frac{1}{\rho} \quad \text{(Bare Coulomb)}$$

and

$$A(k) = \frac{2\pi e^{-ka}}{k} \quad \rightarrow \quad \phi(\rho, z=0) = \frac{1}{\sqrt{\rho^2 + a^2}} \quad \text{(Bare Coulomb from } a \text{ away)}$$

so that $A(k) = (2\pi/k)(e^{-ka} - e^{-kb})$ represents a dipole with positive charge at $z = -a$ and negative charge at $z = -b$ which will create a dipolar field: the signature in k space at small k is linear behavior and the dipole strength shows up as the coefficient of k (after eliminating $2\pi/k$).

For surface charge distributions with cylindrical symmetry, we are talking about integrals like

$$\Sigma(x, y, z) = \int \frac{d^2k}{(2\pi)^2} \tilde{\Sigma}(k, z) e^{ik_x x + ik_y y} = \int_0^\infty dk \, \frac{k}{2\pi} \tilde{\sigma}(k, z) J_0(k\rho)$$

so that the most elementary integral is

$$\tilde{\Sigma}(k, z) = e^{-kd} \quad \rightarrow \quad \Sigma(\rho, z) = \frac{d}{(d^2 + \rho^2)^{3/2}} \, .$$

To understand the above complex expression for A, let's proceed by simple cases.

☐ The first example is to consider a point charge right on the surface of an infinite half space of dielectric. So we set $\tilde{\sigma}_+ = 1$, $\tilde{\sigma}_- = 0$, and send $d_1 \rightarrow \infty$ or $u \rightarrow 0$. This gives

$$A = \frac{2\pi}{k} \cdot \frac{2}{\epsilon_1 + 1} \quad \rightarrow \quad \phi(\rho, z=0) = \frac{1}{\rho(\epsilon_1 + 1)/2} \, .$$

The potential is screened by the average dielectric constant of the two half spaces: unity and ϵ_1. This answer can actually be gotten by symmetry without any Fourier transforms.

☐ Next, consider a point charge above an infinite half-space of dielectric. So we set $\tilde{\sigma}_+ = 1$, $\tilde{\sigma}_- = 0$, and easiest to achieve what we want is to set $\epsilon_1 = 1$ and $d_2 \rightarrow \infty$ so $v \rightarrow 0$. We get

$$A = \frac{2\pi}{k} \cdot \left[1 - \left(\frac{\epsilon_2 - 1}{\epsilon_2 + 1} \right) e^{-2kd_1} \right] \quad \rightarrow \quad \phi(\rho, z=0) = \frac{1}{\rho} - \frac{\frac{\epsilon_2 - 1}{\epsilon_2 + 1}}{\sqrt{\rho^2 + (2d_1)^2}} \, .$$

So we get original point charge plus an image charge d_1 below the surface of the dielectric where the magnitude of the image charge is negative and given by the ratio $(\epsilon_2 - 1)/(\epsilon_2 + 1)$. Obviously for $\rho \gg d_1$ it reduces to the previous case since d_1 becomes irrelevant: from far away, we "can't see" if the charge is right above or on the dielectric.

☐ Now for the problem of a point charge above a finite dielectric slab. Here $\tilde{\sigma}_+ = 1$, $\tilde{\sigma}_- = 0$ and $\epsilon_1 = 1$. We can write this in a few ways

$$\begin{aligned}
A &= \frac{2\pi}{k} \cdot \frac{(1+u)(1-v) + 2\epsilon_2(1+v) + \epsilon_2^2(1-u)(1-v)}{(\epsilon_2+1)^2 - (\epsilon_2-1)^2 v} \\
&= \frac{2\pi}{k} \cdot \frac{(\epsilon_2+1)^2 - (\epsilon_2^2-1)u - (\epsilon_2-1)^2 v + (\epsilon_2^2-1)uv}{(\epsilon_2 + 1 + (\epsilon_2-1)\sqrt{v})(\epsilon_2 + 1 - (\epsilon_2-1)\sqrt{v})} \\
&= \frac{2\pi}{k} \cdot \frac{(1+u)(1-v) + 2\epsilon_2(1+v) + \epsilon_2^2(1-u)(1-v)}{(1-v) + 2\epsilon_2(1+v) + \epsilon_2^2(1-v)} \\
&= \frac{2\pi}{k} \cdot \left[1 - \frac{(\epsilon_2^2-1)(1-v)u}{(\epsilon_2+1)^2 - (\epsilon_2-1)^2 v} \right] .
\end{aligned}$$

This is of the form of the original charge with a negative image charges that have extension in space due to the k dependence. The image charges must be dipolar in form due to the $(1-v)$ form which goes to zero linearly in k as $k \to 0$, and it points the opposite way from the positive point charge due to the negative overall factor in front. In terms of images, the numerator has negative thing at $z = -2d_1$ and an equal positive thing at $z = -2(d_1 + d_2)$ which create the induced dipole.

For $\epsilon_2 \to \infty$ or a metallic slab, we get

$$\lim_{\epsilon_2 \to \infty} A = \frac{2\pi}{k} \cdot (1-u) = \frac{2\pi}{k} \cdot (1 - e^{-2kd_1}) \quad \longrightarrow \quad \phi(\rho, z=0) = \frac{1}{\rho} - \frac{1}{\sqrt{\rho^2 + (2d_1)^2}}$$

which is the classic result of an exactly opposite image charge symmetrically located below the to plane ($2d_1$ below the positive charge). Notice how the thickness of the slab d_2 is completely irrelevant here: this means the positive polarization charge in the metal is smoothed out over the bottom surface as an infinitessimal density over the whole $z = -d_1 - d_2$ plane.

In the opposite limit of a very weak dielectric $\epsilon_2 \to 1$, Taylor series gives

$$A = \frac{2\pi}{k} \cdot \left[1 - \frac{1}{2}(u - uv)(\epsilon_2 - 1) + O((\epsilon_2 - 1)^2) \right]$$

which corresponds to the bare initial charge as well as a polarization (image) charge consisting of a dipole of charges of strength 1/2 with -1/2 charge on the $z = -d_1$ plane and +1/2 on the $z = -d_1 - d_2$ planes scaled by the polarizability $\epsilon_2 - 1$. The dipole points away from the positive charge as it should; the 1/2 strength is because only 1/2 of the electric field lines from the positive point charge point downwards to the dielectric and cause polarization; 1/2 of the field lines pass any $z =$constant plane.

The more generic case of intermediate ϵ_2 is much more complicated: the numerator of A is easily interpreted as charges placed at various z since we have polynomials in u and v with constant coefficients, but the variables v-dependent denominator makes the screening coefficient k dependent so the interpretation is harder. But we can proceed slowly. For very very large ρ, only the region in k satisfying $k\rho \sim 1$ matters in the integral so the relevant k are very small and $kd_2 \ll 1$. Thus setting $v \to 1$, we get

$$\lim_{kd_2 \to 0} A = \frac{2\pi}{k} \cdot 1$$

so we have just the unscreened bare charge: whatever polarizations take place in the dielectric can only give dipolar contributions (net neutral shifting of dielectric charges) which are subleading. A series expansion in $(v-1)$ gives

$$A = \frac{2\pi}{k} \cdot \left[1 + \frac{(\epsilon_2^2 - 1)u(v-1)}{4\epsilon_2} + O((v-1)^2) \right] .$$

What is interesting is that the series as actually converging not just when $v - 1$ is small because $kd_2 \ll 1$ but in addition for large ϵ_2 the correct quantity that must be small is $\epsilon_2(v-1)$ or equivalently $\epsilon_2 kd_2 \ll 1$ (u is between 0 and 1 always so that part is under control). This is the true condition of "small" k or large ρ where the asymptotic limit of seeing the bare point charge is applicable. Translated into ρ via $\rho k \sim 1$, it must be that $\rho \gg \epsilon_2 d_2$ for this limit: only for ρ this large is the dielectric polarization giving a dipole contribution that is negligible (and thus truly dipolar). The mathematical reason for ϵ_2 entering here is that the denominator of A changes very rapidly as a function of v close to $v=1$ for large ϵ_2: it goes from $4\epsilon_2$ at $v=1$ to $(\epsilon_2+1)^2$ for $v=0$ with a slope $-(\epsilon_2-1)^2$ at $v=1$.

A more direct approach is to rewrite the last exact form of A as

$$A = \frac{2\pi}{k} \cdot \left[1 - u + u \cdot \frac{2(1-v) + 2\epsilon_2(1+v)}{(1-v) + 2\epsilon_2(1+v) + \epsilon_2^2(1-v)} \cdot\right]$$

We see the positive and exact negative image as for a metallic system. What is added is a positive image that is weak for $\epsilon_2 \gg 1$. The function multiplying u goes from unity at $k=0$ or $v=1$ to a very small number of order $\sim 1/\epsilon_2$ when v departs significantly from 1 (due to the rapid variation of the denominator). This function drops most of its value for k going from zero to something on the order of $1/(d_2\epsilon_2)$ meaning that in real space this positive image charge must be of extent $\sim d_2\epsilon_2$ in real space. Thus for large ϵ_2 we have the following picture: the positive charges almost an exact negative image surface charge on the top surface at $z=-d_1$ (mathematically behaving as a negative point image charge at $z=-d_2$) and the positive part of the induced polarization charge on the bottom surface at $z=-(d_1+d_2)$ is quite wide in ρ of extent $\epsilon_2 d_2$ and obviously of total magnitude equal to the top surface charge density. So we get a very localized top negative surface charge of extent $\sim d_1$ but the bottom one instead is positive and of size $\sim \epsilon_2 d_2$.

□ Now we get rid of the STO slab, most easily done by setting $\epsilon_2 = 1$. Also let's assume the two charges are exactly equal and opposite distributions in shape so $\tilde{\sigma}_- = -\tilde{\sigma}_+$; a particular example are point charges $\tilde{\sigma}_\pm = \pm 1$. Then we get

$$A = \frac{4\pi}{k} \cdot \frac{\tilde{\sigma}_+(k)(1-e^{-kd_1})}{\epsilon_1 + 1 + (\epsilon_1 - 1)e^{-kd_1}}$$

In the $\rho \to 0$ limit, we concentrate on $k \to \infty$ and we have $A \approx (2\pi/k)(1/(\epsilon_1+1)/2)$ which is just the screened potential of the positive point charge as if on an infinitely thick dielectric. For $\rho \to \infty$, we concentrate on $k \to 0$ where $A \approx (2\pi/k)(1-e^{-kd_1})/\epsilon_1$: this is just a dipole of strength d_1 (positive-negative separation) screened by the dielectric; from far away we just see a screened dipole of the free charges.

□ Here we still set $\epsilon_2 = 1$ but allow for the two charges to be different. We get the more complicated

$$A = \frac{4\pi}{k} \cdot \frac{\tilde{\sigma}_+[\epsilon_1 + 1 + (\epsilon_1 - 1)e^{-2kd_1}] + \tilde{\sigma}_-[2\epsilon_1 e^{-kd_1}])}{(\epsilon_1+1)^2 - (\epsilon_1-1)^2 e^{-2kd_1}}.$$

By linearity, we get the two separate solutions for the positive and negative charge. The denominator, in the limit $k \to 0$ goes to $4\epsilon_1$. So for large ρ and small k we have approximately (after some slight rearrangement)

$$A \approx \frac{2\pi}{k} \cdot \left\{\tilde{\sigma}_+[1 - (\frac{1}{2} - \frac{1}{2\epsilon_1}) + (\frac{1}{2} - \frac{1}{2\epsilon_1})e^{-2kd_1}] + \tilde{\sigma}_- e^{-kd_1}\, .\right\}$$

So there is the bare (unscreened) field of the two free charges as well as an induced opposite dipole created by charges of $(1-1/\epsilon_1)/2$ at $z=0$ and $z=-2d_1$. At long range, this is just gives the screened dipole from the free charges.

☐ We make the STO dielectric constant be very large and go to infinity (a metal). Then we get

$$A = \frac{4\pi}{k} \cdot \frac{\tilde{\sigma}_+[1 - e^{-2kd_1}]}{\epsilon_1 + 1 + (\epsilon_1 - 1)e^{-2kd_1}} .$$

Notice that the negative charge $\tilde{\sigma}_-$ drops out completely: when we put the negative charge on top of the metal, an opposite charge collects right under it and screens it completely. What we have here instead (for large ρ and thus small k) is a screened dipole:

$$A \approx \frac{2\pi}{k} \cdot \frac{\tilde{\sigma}_+[1 - e^{-2kd_1}]}{\epsilon_1} .$$

but while the positive charge is at $z = 0$, the negative charge is exactly opposite and at $z = -2d_1$ as per the classic image problem (case 2 above). So again we get a screened dipole but of twice the physical length $2d_1$. The total dipole is thus $2d_1/\epsilon_1$.

Before concluding this particular example, there is one thing to note. In this metallic case, for a unit positive charge, exactly one unit of negative charge has distributed itself on the upper STO (metal) surface to act as an image charge at $-d_1$ — the polarization charge in the LAO film is net neutral as it is just dipole polarization. However, in the metal, there must be a positive unit of charge somewhere, and for a true metal with infinite dielectric constant it is spread evenly over the entire bottom surface as a infinitessimal surface charge density. When the STO has a finite but large dielectric constant, as in the case above where we studied dielectric STO slab alone more carefully, this approximately one unit of positive charge will be spread over a finite but large distance of $\sim d_2\epsilon_2$ on the bottom surface. What this means is that the field can't be a dipolar one as described above but that when $\rho \gg \epsilon_2 d_2$, this unit of charge will also make a contribution that simply goes as $\approx 1/\rho$. More on this further below.

☐ Say we let the STO become infinitely thick so $d_2 \to \infty$ and $v \to 0$ for any k. A becomes

$$A = \frac{4\pi}{k} \cdot \frac{\epsilon_2\tilde{\sigma}_+(1 - e^{-2kd_1}) + \epsilon_1(\tilde{\sigma}_+ + 2\tilde{\sigma}_- e^{-kd_1} + \tilde{\sigma}_+ e^{-2kd_1})}{(\epsilon_1 + 1)(\epsilon_2 + \epsilon_1) + (\epsilon_1 - 1)(\epsilon_2 - \epsilon_1)e^{-2kd_1}} .$$

For small k, the denominator is $\approx 2\epsilon_1(1 + \epsilon_2)$. This leads to

$$A \approx \frac{2\pi}{k} \cdot \left[\frac{\tilde{\sigma}_+(1 - e^{-2kd_1})}{\epsilon_1(1 + 1/\epsilon_2)} + \frac{\tilde{\sigma}_+ + 2\tilde{\sigma}_- e^{-kd_1} + \tilde{\sigma}_+ e^{-2kd_1}}{1 + \epsilon_2}\right] .$$

In that limit of large ρ, the potential is given by the superposition of two distributions: (i) a dipole formed by $+\sigma_+$ at $z = 0$ and $-\sigma_+$ at $z = -2d_1$ reduced in strength by a factor $\epsilon_1(1 + 1/\epsilon_2)$, and (ii) a quadropolar arrangement of σ_+ at $z = 0$ and $z = -2d_1$ and $2\sigma_-$ at $z = -d_1$ and all three reduced by a factor $(1 + \epsilon_2)$. The dipolar term is dominant for large ρ: we have a screened dipole where screening is due to ϵ_1. The strength of the screened dipole is $2d_1/(\epsilon_1(1 + 1/\epsilon_2))$ which tunes nicely between the no STO $\epsilon_2 = 1$ limit and the metallic STO $\epsilon_2 = \infty$ limits. So whatever dipole it is is screened by ϵ_1, and the value being screened depends on ϵ_2 which changes its length from d_1 to $2d_1$ as ϵ_2 goes from unity to very large.

☐ Take the full blown expression for A and let the positive and negative charge have identical spatial profile: $\tilde{\sigma}_+ = -\tilde{\sigma}_-$. Then for $k \to 0$, we have using the approximate denominator $8\epsilon_1\epsilon_2$ at $k = 0$

$$A \approx \frac{2\pi}{k} \cdot \tilde{\sigma}_+ \cdot \left[\frac{(1 - e^{-kd_1})^2(1 + \epsilon_2 + (\epsilon_2 - 1)e^{-2kd_2})}{4\epsilon_2} + \frac{(1 - e^{-2kd_1})(1 + \epsilon_2 - (\epsilon_2 - 1)e^{-2kd_2})}{4\epsilon_1}\right] .$$

Here we have taken k so small so that we are really in the true far field limit. The first term is quadropolar (either by Taylor expanding in k or by expanding the first square and seeing it term by term) so for the far field we can ignore it. The second term for small k is dipolar with two point charges at $z = 0$ and $z = -2d_1$ of strength $1/(2\epsilon_1)$ which in the end generates a dipole d_1/ϵ_1: just the screened free dipole by only ϵ_1. Again, the effect of ϵ_2 here is weak and even weaker than the case above of infinitely thick STO as it does nothing to the long range dipolar field. The difference is due to the finite thickness of d_2 and that we are in the $\rho \gg d_2$ limit or $kd_2 \ll 1$.

☐ Doing the general case of possibly different σ_+ and σ_-, Taylor expanding everything in sight still gives a monopole of strength $\tilde{\sigma}_+ + \tilde{\sigma}_-$ and a dipole of strength

$$p = -\left(d_1 + d_2 - \frac{d_2}{\epsilon_2}\right) \cdot (\tilde{\sigma}_+ + \tilde{\sigma}_-) + \frac{d_1}{\epsilon_1}\tilde{\sigma}_+ \,.$$

If we set $\tilde{\sigma}_+ + \tilde{\sigma}_- = 0$ as $k \to 0$ then we just recover the previous result of a screened dipole of total strength d_1/ϵ_1. Again, these are extremely large ρ far field limits.

☐ The above two cases have dealt with finite slabs and finite dielectric constants and the truly large ρ limit. What that means is $\rho \gg d_2\epsilon_2$ where all the polarization charges are truly "exhausted" as dipoles. We should keep in mind that for large but smaller ρ, the contribution from the surface charge density on the bottom STO surface $z = -d_1 - d_2$ will not be in its asymptotic limit as on still "inside" the distribution. See below for implications.

For completeness, the potential on the $z = -d_1$ plane where the negative charge is located is given by $A_1/\sqrt{u} + B_1\sqrt{u}$ that equals

$$\frac{4\pi}{k}\cdot\frac{[2\epsilon_1\tilde{\sigma}_+\sqrt{u} + \tilde{\sigma}_-(1+\epsilon_1+(\epsilon_1-1)u)][1+\epsilon_2+(\epsilon_2-1)v)]}{\epsilon_2(1-u)(\epsilon_2(1-v)+v+1)+\epsilon_1^2(1-u)(1+\epsilon_2+(\epsilon_2-1)v)+\epsilon_1(1+u)((1+\epsilon_2)^2-(\epsilon_2-1)^2v)}\,.$$

As expected, this expression goes to zero for $\epsilon_2 \to \infty$ since we're asking for the potential on the metal surface which must be zero.

Some numerical results are in order. To do this, set $\epsilon_2 = 300$, $\epsilon_1 = 30$, and assume for simplicity that $d = d_1 = d_2$ or $u = v$. This yields

$$A = \frac{4\pi}{k}\cdot\frac{2\tilde{\sigma}_- e^{-kd}(301+299e^{-2kd}) + \tilde{\sigma}_+(3311-5400e^{-2kd}+3289e^{-4kd})}{102641-4860e^{-2kd}-95381e^{-4kd}}\,.$$

and

$$\frac{A_1}{\sqrt{u}} + B_1\sqrt{u} = \frac{4\pi}{k}\cdot\frac{[301+299e^{-2kd}][2\tilde{\sigma}_+e^{-kd}+\tilde{\sigma}_-(1.033+0.9667e^{-2kd})]}{102641-4860e^{-2kd}-95381e^{-4kd}}\,.$$

More practical expressions are

$$A = \frac{2\pi}{k}\cdot\frac{\tilde{\sigma}_+(0.0694268-0.11323e^{-2kd}+0.0689655e^{-4kd}) + \tilde{\sigma}_- e^{-kd}(0.0126231+0.0125392e^{-2kd})}{(1.0122-e^{-2kd})(1.06315+e^{-2kd})}$$

and

$$\frac{A_1}{\sqrt{u}}+B_1\sqrt{u}=\frac{2\pi}{k}\cdot\frac{\tilde{\sigma}_+e^{-kd}(0.0126231+0.0125392e^{-2kd})+0.00606061\tilde{\sigma}_-(1.00669+e^{-2kd})(1.06897+e^{-2kd})}{(1.0122-e^{-2kd})(1.06315+e^{-2kd})}$$

Numerical integration of A to give $\phi(\rho, z=0)$ for the positive point charge case $\tilde{\sigma}_+ = 1$ and $\tilde{\sigma}_- = 0$ in units of $d_1 = d_2 = d = 1$ (i.e. what is tabulated is $d\phi(\rho, z=0)$) gives

ρ	Actual Integral	$[\rho(\epsilon_1+1)/2]^{-1}$	Integral with $\epsilon_2=\infty$	Integral with $d_2=\infty$	$\left[\rho^2+100^2\right]^{-\frac{1}{2}}$	$1/\rho$
0.01	6.44	6.45	6.41	6.41	1.00×10^{-2}	100
0.1	0.632	0.645	0.601	0.607	1.00×10^{-2}	10
1.0	5.57×10^{-2}	6.45×10^{-2}	2.63×10^{-2}	3.15×10^{-2}	1.00×10^{-2}	1
10	1.80×10^{-2}	6.45×10^{-3}	2.39×10^{-6}	6.74×10^{-4}	9.95×10^{-3}	0.1
50	9.43×10^{-3}		1.78×10^{-8}	1.33×10^{-4}	8.94×10^{-3}	2.00×10^{-2}
100	6.39×10^{-3}		2.22×10^{-9}	6.65×10^{-5}	7.07×10^{-3}	1.00×10^{-2}
300	2.89×10^{-3}				3.16×10^{-3}	3.33×10^{-3}
500	1.86×10^{-3}				1.96×10^{-3}	2.00×10^{-3}
1000	9.77×10^{-4}				9.95×10^{-4}	1.00×10^{-3}
5000	2.00×10^{-4}				2.00×10^{-4}	2.00×10^{-4}

The logic for the column $\left[\rho^2+100^2\right]^{-\frac{1}{2}}$ is that in the limit of almost metallic screening of large ϵ_2 for STO, we expect about -1 unit of image charge acting as in the $\epsilon_2=\infty$ case that forms a dipolar field but in addition a positive unit charge is spread out on the bottom STO surface over a length scale of $\sim d\epsilon_2$. The actual number 100 is a bit arbitrary but just has the right order of magnitude. Any large such number gives the correct asymptotic result of $1/\rho$ for ρ large enough; the point is that that limit gets approached as $\rho \sim d\epsilon_2$. The table shows that actually the sum of the metallic $\epsilon_2=\infty$ plus this additional bottom charge gives a total good and reasonable result compared to the actual integral.

Similar numerical integration of $A_1/\sqrt{u}+B_1\sqrt{u}$ for $\phi(\rho, z=-d_1)$ with $\tilde{\sigma}_+=1$ and $\tilde{\sigma}_-=0$ gives

ρ/d	Integral
0	0.0349
0.1	0.0348
0.5	0.0336
1.0	0.0312
2.0	0.0274
3.0	0.0250
5.0	0.0220
10	0.0180
20	0.0141
30	0.0120
40	0.0105
50	0.00944
100	0.00639

Again, the field has two parts: for ρ large, it is again due to the bottom STO charge. For small ρ, we get the almost dipolar contribution of (zero) at the plane plus something scaling as $1/\epsilon_2$ due to imperfect metallicity.