Composition and refractive index calibration of co-deposited TiO_2/SiO_2 films via sputtering

In this Teaching Module, we determine the composition required for a certain refractive index (n) of a co-sputtered film deposited by two different sputtering target materials. The refractive index of a co-sputtered film is based upon the volume fraction ratio of one sputtered target material to the other, which is dependent upon the deposition rate of each of the materials. For these calculations we assume that growth rate varies linearly with RF power, while operating pressure, temperature, and argon and oxygen flow rates are assumed to be constant during the sputtering process.

Model based on percentage volume growth rates

For our discussion we make the assumption that the growth rate of a sputtered film is linearly dependent on the power supplied to the target expressed as

$$GR_{\text{target}} = a_{\text{target}}\, P_{\text{target}}, \tag{1}$$

where GR_{target} is growth rate of the target in nm min^{-1}, a_{target} is a constant for the sputtering target, and P_{target} is the power supplied to the target. Rewriting eq. (1) for SiO_2 and TiO_2 we obtain

$$a_{\text{SiO2}} = \frac{GR_{\text{SiO2}}}{P_{\text{SiO2}}}, \tag{2}$$

$$a_{\text{TiO2}} = \frac{GR_{\text{TiO2}}}{P_{\text{TiO2}}}. \tag{3}$$

Initially in this model we will hold the co-sputtered film growth rate fixed in order to ease calculations. This rate is determined by the upper growth rate limit (GR_{lim}) of the “slower” target, i.e. TiO_2.

$$GR_{\text{lim}} \equiv GR_{\text{TiO2\_max}}, \tag{4}$$

where $GR_{\text{TiO2\_max}}$ is the maximum achievable growth rate for the TiO_2 target. Therefore, GR_{lim} for the co-sputtered film can also be expressed as

$$GR_{\text{lim}} = GR_{\text{SiO2}} + GR_{\text{TiO2}}, \tag{5}$$

where GR_{SiO2} and GR_{TiO2} are growth rates for the SiO_2 and TiO_2 targets, respectively. By substituting Eq. (1) into Eq. (5) we now have a formula relating co-deposited film growth rate with individual target materials and corresponding powers

$$GR_{\text{lim}} = a_{\text{SiO2}}\, P_{\text{SiO2}} + a_{\text{TiO2}} P_{\text{TiO2}}. \tag{6}$$

The volume, V, grown by a co-deposited film is

$$V_{\text{film}} = V_{\text{SiO2}} + V_{\text{TiO2}}. \tag{7}$$

Because the area and time of the deposition are identical for the two targets, the volume is given by

$$V_{\text{target}} = GR_{\text{target}}\, A\, t, \tag{8}$$

where A is deposition area (wafer area) and t the growth time. The refractive index, n, for a TiO_2/SiO_2 co-deposited film, can now be expressed using the composition of SiO_2 and TiO_2

$$n_{\text{TiO2\_SiO2}} = \frac{V_{\text{TiO2}} n_{\text{TiO2}} + V_{\text{SiO2}} n_{\text{SiO2}}}{V_{\text{film}}}, \tag{9}$$

or,

$$n_{\mathrm{TiO2\_SiO2}} = n_{\mathrm{TiO2}}\, x + n_{\mathrm{SiO2}}\, (1 - x), \tag{10}$$

where x the compositional fraction of TiO_2 in the film which is described by

$$x = \frac{V_{\mathrm{TiO2}}}{V_{\mathrm{TiO2}} + V_{\mathrm{SiO2}}} = \frac{P_{\mathrm{TiO2}}}{P_{\mathrm{TiO2}} + \frac{a_{\mathrm{SiO2}}}{a_{\mathrm{TiO2}}} P_{\mathrm{SiO2}}} = \frac{(n_{\mathrm{TiO2\_SiO2}} - n_{\mathrm{SiO2}})}{(n_{\mathrm{TiO2}} - n_{\mathrm{SiO2}})}, \tag{11}$$

The co-sputtered film TiO_2 volume fraction verses refractive index is shown in Fig. 1.

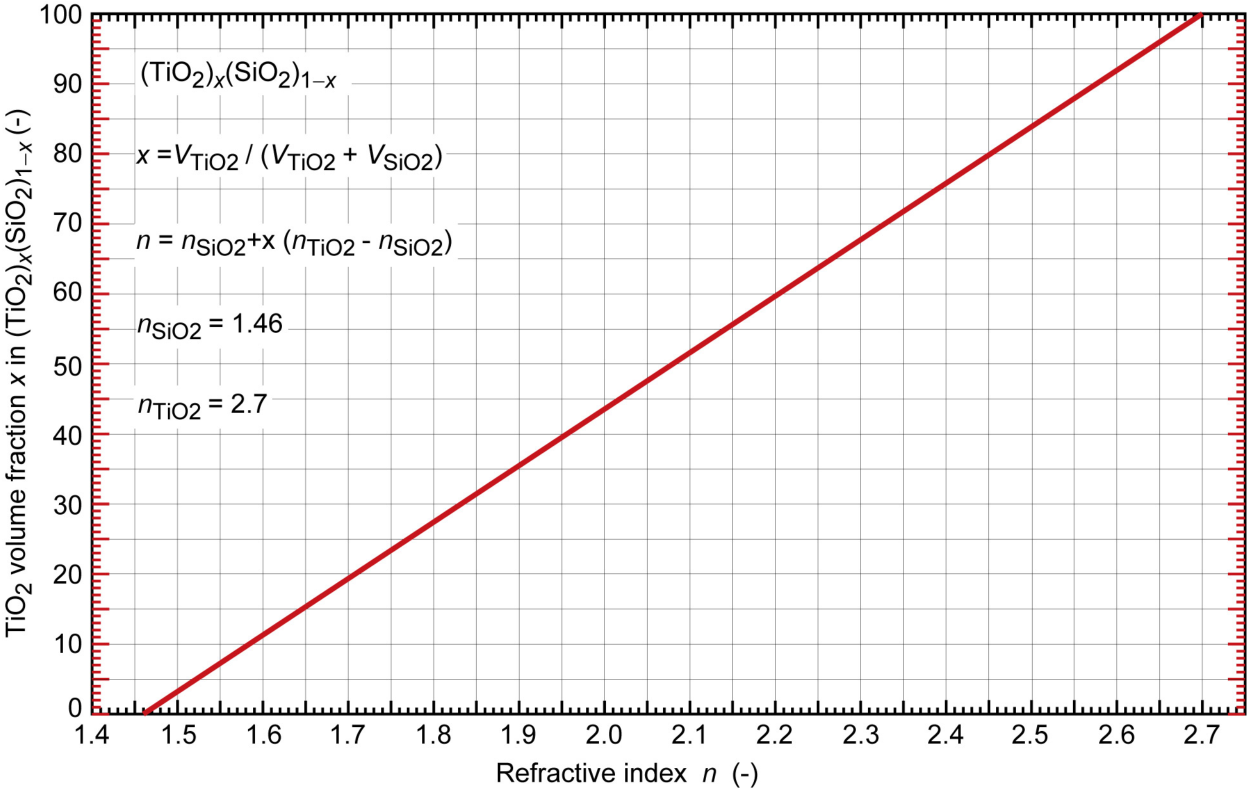

Fig. 1: Relative composition x of TiO_2 in $(TiO_2)_x(SiO_2)_{1-x}$ as a function of the refractive index.

For a given $n_{\mathrm{TiO2\_SiO2}}$ and inserting Eq. (11) into (12), we now calculate P_{TiO2} as

$$P_{\mathrm{TiO2}} = x\, P_{\max}\,, \tag{12}$$

Similarly the power P_{SiO2} is calculated as

$$P_{\mathrm{SiO2}} = (1 - x)\, \frac{a_{\mathrm{SiO2}}}{a_{\mathrm{TiO2}}}\, P_{\max}, \tag{13}$$

thereby predicting TiO_2 and SiO_2 powers for any desired index. Fig. 2 shows P_{TiO2} and P_{SiO2} as a function of volume fraction x of TiO_2 with a range of ratios in TiO_2 to SiO_2.

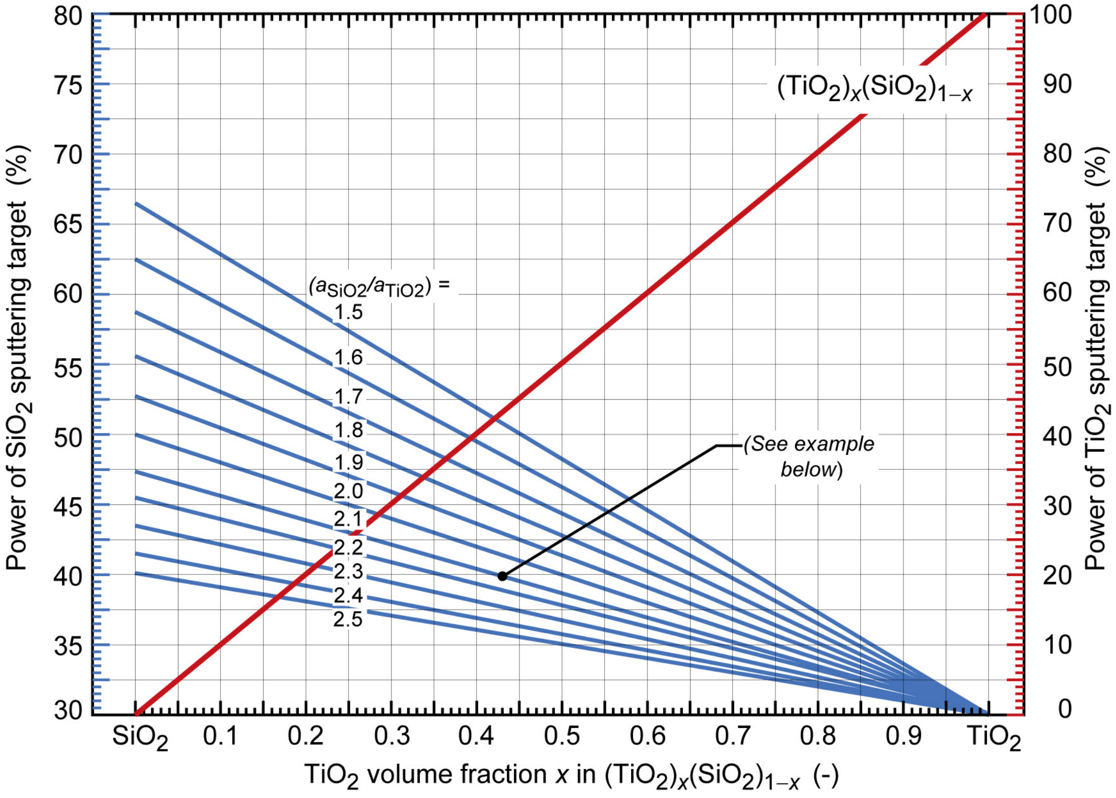

Fig. 2: TiO_2 and SiO_2 sputter power as a function TiO_2 volume fraction plotted with a range of values in the growth rate ratio SiO_2 to TiO_2.

Example calibration of co-sputtered TiO_2/SiO_2 film with constant growth rate

For example, we consider a hypothetical case, Fig. 3, setting $a_{SiO2} = 0.015$ nm min^{-1}, $a_{TiO2} = 0.007$ nm min^{-1}, $GR_{lim} = 1.4$ nm min^{-1}, and $n_{SiO2} = 1.45$, $n_{TiO2} = 2.6$. $a_{SiO2} / a_{TiO2} = 2.14 \approx 2.1$ (see figure above).

Note: For this model we are using a constant growth rate (independent of x), i.e. the rate of the slower target. For many applications this is not as desirable as using maximum growth rate. It is possible to obtain the maximum growth rate by utilizing the above derivations. Start by finding the powers required for each target for a given refractive index assuming constant growth rate, then shifting the limiting power supply up to its maximum power and the other target by the corresponding amount as given by Eq. (12) and (13).