# New Amorphous Dispersion Formula

Spectroscopic ellipsometry (SE) is a technique based on the measurement of the relative phase change of reflected and polarized light in order to characterize thin film optical functions and other properties. The measured data are used to describe a model where each layer refers to a given material. The model uses mathematical relations called dispersion formulae that help to evaluate the material's optical properties by adjusting specific fit parameters.

This application note deals with the new amorphous dispersion formula. For further information about the original theory derived from Forouhi-Bloomer, please refer to the technical note «Forouhi Bloomer alias Amorphous dispersion formula».

## New Amorphous theoretical model

The «New Amorphous» dispersion formula was derived by Horiba Jobin Yvon on the basis of Forouhi-Bloomer formulation. This new formulation was established in order to give a Lorentzian shape to the expressions of the extinction coefficient and refractive index. The absorption coefficient is given by :

$$k(\omega)=\begin{cases}\dfrac{f_j\cdot(\omega-\omega_g)^2}{(\omega-\omega_j)^2+\Gamma_j^2} & ;\text{for } \omega>\omega_g \\ 0 & ;\text{for } \omega\le\omega_g\end{cases} \quad (1)$$

The refractive index is written through this formula :

$$n(\omega)=n_\infty+\frac{B\cdot(\omega-\omega_j)+C}{(\omega-\omega_j)^2+\Gamma_j^2} \quad (2)$$

where :

$$\begin{cases}B_j=\dfrac{f_j}{\Gamma_j}\cdot\left(\Gamma_j^2-(\omega_j-\omega_g)^2\right) \\ C_j=2\cdot f_j\cdot\Gamma_j\cdot(\omega_j-\omega_g)\end{cases} \quad (3)$$

## Extension to multiple oscillators: «N - New Amorphous»

The New Amorphous formulation can be extended to the case where many oscillators are present in the material. Such dispersions are called « N – New Amorphous » and are given in the array below.

| Formula | Number of oscillators | Number of parameters |
|---|---|---|
| New Amorphous | N=1 | 5 |
| Double New Amorphous | N=2 | 8 |
| Triple New Amorphous | N=3 | 11 |

The equations for k(ω) and n(ω) for N oscillators are given below :

- for the extinction coefficient :

$$k(\omega)=\begin{cases}\displaystyle\sum_{j=1}^{N}\frac{f_j\cdot(\omega-\omega_g)^2}{(\omega-\omega_j)^2+\Gamma_j^2} & ;\text{for } \omega>\omega_g \\ 0 & ;\text{for } \omega\le\omega_g\end{cases} \quad (4)$$

- for the refractive index :

$$n(\omega)=n_\infty+\sum_{j=1}^{N}\frac{B_j\cdot(\omega-\omega_j)+C_j}{(\omega-\omega_j)^2+\Gamma_j^2} \quad (5)$$

Increasing the number of oscillators leads to a shift of the peaks of absorption toward the ultraviolet region.

## The parameters of the equation

### Parameter describing the refractive index

The term n(∞) is an additional parameter, at least greater than one and equal to the value of the refractive index when $\omega \to \infty$.

4 parameters describe the extinction coefficient.

- $f_j$ ($j$=1, 2, 3) (in eV) is related to the strength (amplitude) of the extinction coefficient peak. As the value of $f_j$ increases both values of the refractive index and extinction coefficient increases. Generally, $0<f_j<1$.
- $\Gamma_j$ ($j$=1, 2, 3) (in eV) is the broadening term of the peak of absorption. The larger $\Gamma_j$ is the larger the absorption peak but the smaller its amplitude. Generally, $0.2<\Gamma_j<8$.
- $\omega_j$ (in eV) is approximately the energy at which the extinction coefficient is maximum (peak of absorption). As the value of $\omega_j$ increases the absorption peak is shifted towards the UV region. Generally, $1.5<\omega_j<10$.
- $\omega_g$ (in eV) is the energy band gap. It is equal to the minimum of energy required for a transition from the valence band to the conduction band. It is the energy from which the absorption starts to be non-zero: $k(E \geq Eg) \geq 0$. Always, $\omega_g < \omega_j$.

### Relations between «Amorphous» and «New Amorphous» parameters

The array below gives the relations between the parameters of Forouhi-Bloomer and New Amorphous dispersion formulae.

| Forouhi-Bloomer | New Amorphous |
|---|---|
| $A$ | $f_j$ |
| $B$ | $2.\omega_j$ |
| $C$ | $\omega^2_j+\Gamma^2_j$ |
| $\sqrt{\varepsilon_\infty}$ | $n_\infty$ |
| $E_g$ | $\omega_g$ |

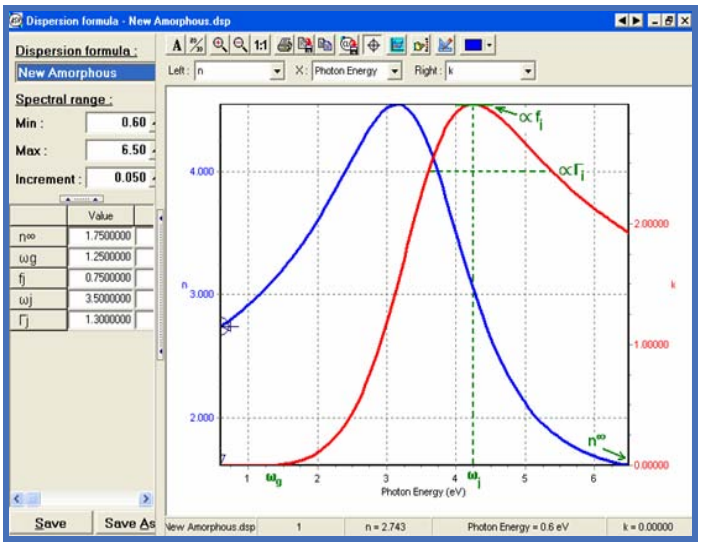
N.B: In DeltaPsi2 software, the user is advised to perform fitting using the «New Amorphous» formula (and its extensions) instead of the «Amorphous» one because $B$ and $C$ parameters are often correlated.

## Parameter setup

Note that :

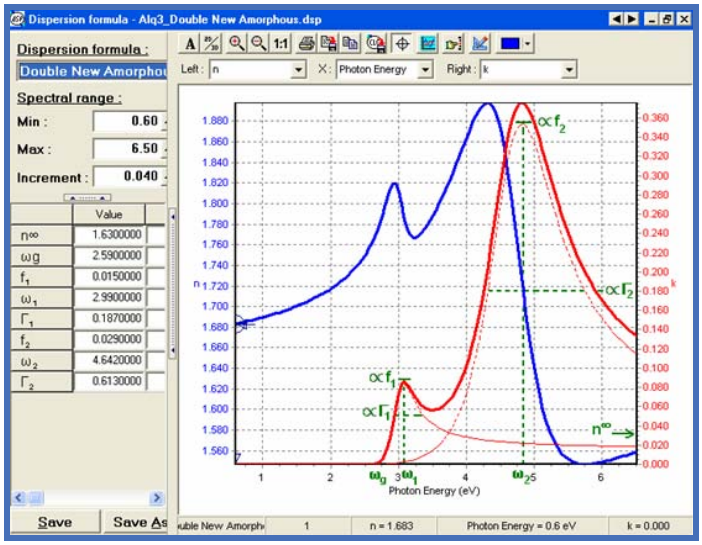
- The graphs below show the different contributions (in red dashed lines) to the imaginary part of the Double New Amorphous dielectric function (in red bold line).
- The sign « $\propto$ » before a given parameter means that either the amplitude or the broadening of the peak is linked to that parameter.

### New Amorphous function




*Optical properties of amorphous silicon given by the New Amorphous function*

### Double New Amorphous function




*Optical properties of Alq3 given by the Double New Amorphous function*

## Applications to materials

The new amorphous model works particularly well for amorphous materials exhibiting an absorption in the visible and/or FUV range (absorbing dielectrics, semiconductors, polymers).

We advise the user to compare the results obtained between the new amorphous and Tauc-Lorentz dispersion formula. The Tauc-Lorentz model may fit better the absorption part of the experimental spectrum.

## Materials following the New Amorphous model

The asterisk * refers to parameters that are negative and thus do not have any physical meaning but represent good starting values to perform the fit on the material.

| Materials | n∞ | $\omega_g$ | $f_j$ | $\omega_j$ | $\Gamma_j$ | S. R. (eV) |
|---|---|---|---|---|---|---|
| **a-C** | 1.564 | 0.542 | 0.123 | 3.620 | 2.645 | 1.5 - 3.5 |
| **AlGaAs** | 1.123 | 4.170 | 2.192 | 5.569 | 0.510 | 0.6 - 3 |
| **$Al_2O_3$** | 1.56 | 9.85 | 2.46 | 10.4 | 0.44 | 0.73 - 4.73 |
| **AlN** | 1.574 | 0.490 | 0.558 | 5.604 | 7.897 | 1.5 - 5 |
| **Alq3** | 1.526 | 0.422 | 0.061 | 8.465 | 2.278 | 0.75 - 4 |
| **Amino-Silane** | 1.298 | 1.342 | 0.181 | 4.659 | 3.166 | 1.5 - 6 |
| **a-Si** | 1.750 | 1.250 | 0.750 | 3.5 | 1.3 | 1.5 - 5 |
| **p-Si** | 2.626 | 0.599 | 0.123 | 3.908 | 0.510 | 1.5 - 5 |
| **AsSe** | 2.499 | 1.686 | 0.242 | 2.471 | 0.562 | 0.75 - 4.5 |
| **AZO** | 1.923 | 2.828 | 0.134 | 3.575 | 0.516 | 0.6 - 2 |
| **$Ba_{0.5}Sr_{0.5}TiO_3$** | 1.843 | 3.702 | 0.256 | 4.892 | 0.940 | 1.5 - 5.5 |
| **$BaTiO_3$** | 1.500 | 3.000 | 0.100 | 5.000 | 0.500 | 1.5 - 5.5 |
| **BaFeO** | 2.538 | 0.936 | 0.022 | 2.374 | 0.213 | 0.75 - 4.7 |
| **BK7** | 1.456 | 5.500 | 0.073 | 8.127 | 1.347 | 1.5 - 5.5 |
| **Ge doped CH** | 3.270 | -3.336* | 0.010 | 2.550 | 0.245 | 1.5 - 6 |
| **CH** | 1.650 | 0.488 | 0.084 | 3.443 | 1.839 | 0.7 - 3 |
| **CFx** | 1.361 | 2.108 | 0.023 | 4.299 | 1.186 | 0.7 - 4.75 |
| **DLC** | 1.501 | 0.420 | 0.093 | 2.783 | 2.237 | 0.75 - 4.75 |
| **Organic EL/HTL** | 0.580 | -1.104* | 0.222 | 11.552 | 4.026 | 0.75 - 4 |
| **Fe oxide** | 1.787 | 0.510 | 0.179 | 3.282 | 1.149 | 0.75 - 4.75 |
| **GaN** | 2.145 | 2.620 | 0.048 | 4.298 | 0.290 | 0.65 - 3 |
| **$GeO_2$** | 1.576 | 1.172 | 0.199 | 1.262 | 6.064 | 0.75 - 2 |
| **Glass** | 1.130 | 3.428 | 0.009 | 16.953 | 0.282 | 0.65 - 5 |
| **Glass 1737** | 0.626 | 3.238 | 0.0549 | 41.765 | 2.309 | 1.5 - 6.5 |
| **$HfO_2$** | 1.436 | 4.831 | 0.259 | 12.138 | 2.718 | 0.75 - 4.5 |
| **InN** | 2.200 | 1.900 | 0.200 | 2.250 | 0.250 | |
| **$In_xGa_{1-x}N$** | 1.857 | -6.448* | 0.006 | 4.915 | 0.762 | 0.75 - 3 |
| **$In_2O_3$** | 1.526 | 3.429 | 0.111 | 3.631 | 0.484 | 1.5 - 5 |
| **$LiAlO_3$** | 2.139 | -12.354* | 0.003 | 2.533 | 0.518 | |
| **$LiNbO_3$** | 2.149 | 4.183 | 0.478 | 4.902 | 0.556 | 1.5 - 5 |
| **MoSi** | 2.089 | -5.109* | 0.172 | 2.928 | 4.385 | 0.75 - 4.5 |
| **LPCVD Nitride** | 1.834 | 2.192 | 0.164 | 5.412 | 2.170 | 1.5 - 4.7 |
| **NPD** | 1.781 | 2.763 | 0.054 | 3.374 | 0.318 | 0.75 - 4 |

| Materials | n∞ | $\omega_g$ | $f_1$ | $\omega_1$ | $\Gamma_1$ | S. R. (eV) |
|---|---|---|---|---|---|---|
| **e-PEDOT-PSS** | 1.563 | 4.149 | 0.0027 | 5.163 | 0.152 | 0.8 - 5.4 |
| **o-PEDOT-PSS** | 1.471 | 3.374 | 0.025 | 6.542 | 0.773 | |
| **PI** | 1.485 | 3.604 | 0.092 | 5.375 | 1.322 | 1.5 - 6.5 |
| **Photoresist** | 1.557 | 1.301 | 0.011 | 5.352 | 0.490 | 1.5 - 6.5 |
| **Polymer** | 1.660 | 0.875 | 0.0434 | 2.435 | 0.442 | 0.6 - 4 |
| **PMMA** | 1.456 | 3.667 | 0.130 | 4.212 | 7.144 | 0.6 - 6 |
| **e - PPV** | 1.516 | 2.878 | 0.0832 | 3.144 | 0.126 | 0.8 - 5.3 |
| **o-PPV** | 1.538 | 1.766 | 0.0763 | 2.383 | 0.241 | |
| **PZT** | 2.345 | 3.000 | 0.183 | 4.350 | 0.424 | 0.6 - 4.7 |
| **Resist** | 1.537 | 2.629 | 0.00364 | 5.312 | 0.079 | 1.5 - 3 |
| **SiGeC** | 3.023 | 0.500 | 0.100 | 4.000 | 0.900 | 0.8 - 3 |
| **$SiN_x$** | 2.071 | 4.388 | 0.657 | 5.288 | 2.848 | 1.5 - 6.5 |
| **$SiN_x$** | 1.750 | 3.420 | 0.160 | 7.310 | 1.700 | 0.75 - 4.5 |
| **$Si_3N_4$** | 1.794 | 2.221 | 0.031 | 7.340 | 0.623 | 0.75 - 4.75 |
| **SiO** | 1.500 | 2.362 | 0.0841 | 5.878 | 1.561 | 0.6 - 6 |
| **TAC** | 1.448 | 2.947 | 0.0507 | 5.244 | 1.966 | 1.5 - 4 |
| **$Ta_2O_5$** | 1.788 | 3.892 | 0.225 | 5.170 | 0.700 | 1.4 - 5 |
| **$TeO_2$** | 2.096 | 2.952 | 0.278 | 4.282 | 0.652 | 0.75 - 4 |
| **$TiO_2$** | 2.096 | 2.952 | 0.278 | 4.282 | 0.652 | 0.75 - 4 |
| **$TiVO_x$** | 1.879 | 1.479 | 0.124 | 3.848 | 0.849 | 0.75 - 4 |
| **$WO_3$** | 1.818 | 2.199 | 0.025 | 4.734 | 0.325 | 1.5 - 4.5 |
| **$WO_x$** | 2.646 | 2.952 | 0.802 | 3.105 | 1.011 | 1.5 - 4.5 |
| **$ZnO_x$** | 1.405 | 2.737 | 0.102 | 3.385 | 0.305 | 1.5 - 4 |
| **$ZnO_2$** | 1.852 | 3.062 | 0.127 | 3.372 | 0.218 | 1.5 - 4 |

## Materials following the Double New Amorphous model

| Materials | n∞ | $\omega_g$ | $f_1$ | $\omega_1$ |
|---|---|---|---|---|
| **Alq3** | 1.630 | 2.590 | 0.029 | 4.642 |
| **AZO** | 1.605 | 1.825 | 0.001 | 3.520 |
| **EIL** | 1.329 | 0.376 | 0.0203 | 5.420 |
| **EML** | 1.329 | 0.376 | 0.0203 | 5.420 |
| **ETL** | 1.702 | 2.881 | 0.0979 | 2.976 |
| **FeCo oxide** | 1.266 | 0.524 | 0.142 | 2.230 |
| **Blue Filter** | 1.616 | 1.463 | 0.0333 | 1.620 |
| **Ge** | 2.389 | -0.918* | 0.366 | 4.436 |
| **HIL** | 1.695 | 2.695 | 0.135 | 3.275 |
| **HTL** | 1.702 | 2.658 | 0.097 | 3.201 |
| **$In_2O_3$** | 1.427 | 3.047 | 0.020 | 4.922 |
| **ITO** | 1.555 | 2.866 | 0.777 | 3.385 |
| **LaTeMnO** | 1.650 | 0.227 | 0.049 | 4.307 |
| **NPD** | 1.717 | 2.893 | 0.066 | 3.167 |
| **p-Si** | 1.800 | 2.250 | 0.550 | 3.250 |
| **TPD** | 1.571 | 2.515 | 0.00723 | 3.933 |
| **Varnish** | 1.604 | -0.519* | 0.053 | -1.662* |

| Materials | $\Gamma_1$ | $f_2$ | $\omega_2$ | $\Gamma_2$ | S. R. (eV) |
|---|---|---|---|---|---|
| **Alq3** | 0.613 | 0.015 | 2.990 | 0.187 | 0.75 - 4 |
| **AZO** | 0.176 | 0.022 | 4.126 | 0.761 | |
| **EIL** | 0.385 | 0.003 | 3.031 | 0.169 | 0.8 - 4 |
| **EML** | 0.385 | 0.003 | 3.031 | 0.169 | 0.8 - 4 |
| **ETL** | 0.100 | -0.060* | 3.398 | -0.538* | 0.8 - 4 |
| **FeCo oxide** | 0.976 | 0.905 | 0.346 | -0.016* | 0.75 - 4 |
| **Blue Filter** | 0.0634 | 0.00588 | 1.928 | 0.117 | 0.7 - 2 |
| **Ge** | 1.862 | 0.003 | 2.248 | 0.119 | 0.8 - 2 |
| **HIL** | 0.369 | 0.0109 | 3.688 | 0.229 | 0.8 - 4 |
| **HTL** | 0.298 | 0.0071 | 3.604 | 0.167 | 0.8 - 4 |
| **$In_2O_3$** | 0.740 | 0.049 | 4.049 | 0.662 | 1.5 - 5 |
| **ITO** | 0.230 | 0.003 | 5.025 | 0.075 | 0.8 - 4 |
| **LaTeMnO** | 0.771 | 0.059 | 1.815 | 0.459 | |
| **NPD** | 0.185 | 0.031 | 3.493 | 0.232 | 0.75 - 4 |
| **p-Si** | 0.450 | 0.250 | 4.250 | 0.500 | |
| **TPD** | 0.232 | 0.0206 | 3.440 | 0.202 | |
| **Varnish** | 0.201 | 0.001 | 6.367 | 0.654 | 1.5 - 6.5 |

## References

1. E. D. Palik, Handbook of Optical Constants of Solids II, Chap. 7.
2. A. R. Forouhi, I. Bloomer, Phys. Rev. B 34, 7018-7026 (1986).
3. A. R. Forouhi, I. Bloomer, Phys. Rev. B 38, 1865 (1988).
4. G.E Jellison, F. A. Modine, Phys. Rev. , 69(3), 371-374 (1996).

Materials following the Triple New Amorphous model

| Materials | $n_\infty$ | $\omega_g$ | $f_1$ | $\omega_1$ | $\Gamma_1$ | $f_2$ |
|---|---|---|---|---|---|---|
| **CuPc** | 1.300 | 1.000 | 0.003 | 1.700 | 0.050 | 0.002 |
| **PET** | 1.653 | 2.216 | 0.00036 | 4.174 | 0.133 | 0.0095 |
| **Poly-carbonate** | 1.000 | 3.500 | 0.010 | 4.500 | 0.200 | 0.100 |
| **ARC coating Polymer** | 1.565 | 4.373 | 0.00289 | 5.451 | 0.189 | 0.0316 |
| **Photoresist** | 1.480 | 3.980 | 0.00048 | 5.426 | 0.0536 | 0.0046 |

| Materials | $\omega_2$ | $\Gamma_2$ | $f_3$ | $\omega_3$ | $\Gamma_3$ | S. R. (eV) |
|---|---|---|---|---|---|---|
| **CuPc** | 2.000 | 0.050 | 0.020 | 3.750 | 0.479 | 0.6 - 4 |
| **PET** | 5.018 | 0.303 | 0.00704 | 6.421 | 0.339 | 1.5 - 6.5 |
| **Poly-carbonate** | 5.500 | 1.000 | 0.050 | 6.300 | 1.000 | 1.5 - 6.5 |
| **ARC coating Polymer** | 4.385 | 0.0204 | 0.0248 | 6.363 | 0.455 | 1.5 - 6.5 |
| **Photoresist** | 4.397 | 0.115 | 0.0242 | 6.453 | 0.366 | 1.5 - 6.5 |