Nonlinear Dielectric $d$-Tensor

For second-order nonlinear susceptibilities in the Cartesian coordinate system:

$$P_{i}^{NL} = \sum_{j,k} \varepsilon_{0} \chi_{i,j,k}^{(2)} E_{j} E_{k}$$

$\chi_{i,j,k}^{(2)}$ in general has 27 independent coefficients (3x3x3=27 for a 3 dimensional tensor). Taking into account the permutation symmetry condition, the order of $E_{j}$ and $E_{k}$ in equation $P_{i}^{NL} = \sum_{j,k} \varepsilon_{0} \chi_{i,j,k}^{(2)} E_{j} E_{k}$ is not important (i.e. $\chi_{i,j,k}^{(2)} = \chi_{i,k,j}^{(2)}$); the number of independent coefficients will be reduced to 18. For convenience, we can define a two dimensional (6x3) nonlinear dielectric tensor, commonly known as Kleinman $d$-tensor:

$$\begin{pmatrix}
    P_{x} \\
    P_{y} \\
    P_{z}
\end{pmatrix} = \varepsilon_{0} \begin{pmatrix}
    d_{11} & d_{12} & d_{13} & d_{14} & d_{15} & d_{16} \\
    d_{21} & d_{22} & d_{23} & d_{24} & d_{25} & d_{26} \\
    d_{31} & d_{32} & d_{33} & d_{34} & d_{35} & d_{36}
\end{pmatrix} \begin{pmatrix}
    E_{x}^2 \\
    E_{y}^2 \\
    E_{z}^2 \\
    E_{x} E_{y} E_{z} \\
    2E_{y} E_{x} E_{z} \\
    2E_{y} E_{z} E_{x}
\end{pmatrix}$$

One obvious advantage of $d$-tensor format is that the full tensor can be written in a two-dimensional matrix; otherwise it would be difficult to express a three-dimensional tensor on a paper. With $d$-tensor, one can derive the strength of nonlinear interacting process in a dielectric medium under electrical field ($E$).

In practical situation, depending on the crystal class, many tensor components actually can be reduced to zero for crystal structure symmetry reason. For example, the $d$-tensor of LiNbO$_3$ (which is triangular 3m crystal class) can be expressed as

$$\begin{pmatrix}
    P_{x} \\
    P_{y} \\
    P_{z}
\end{pmatrix} = \varepsilon_{0} \begin{pmatrix}
    0 & 0 & 0 & 0 & 0 & 0 \\
    -d_{22} & 0 & 0 & d_{31} & 0 & 0 \\
    d_{31} & d_{31} & d_{33} & 0 & 0 & 0
\end{pmatrix} \begin{pmatrix}
    E_{x}^2 \\
    E_{y}^2 \\
    E_{z}^2 \\
    E_{x} E_{y} E_{z} \\
    2E_{y} E_{x} E_{z} \\
    2E_{y} E_{z} E_{x}
\end{pmatrix}$$
Where the nonlinear d coefficient is $d_{22} = 2.59 \text{ pm/V}$, $d_{31} = 4.85 \text{ pm/V}$, and $d_{33} = 25.3 \text{ pm/V}$. Thus, in the case of LiNbO$_3$, when input fundamental wave $E_z(\omega)$ interacts with nonlinear dielectric medium along the selected z-axis through largest nonlinearity $d_{33}$, the induced polarization $P_z$ can be expressed as

$$
\begin{pmatrix}
P_x \\
P_y \\
P_z
\end{pmatrix} = \varepsilon_0 \begin{pmatrix}
0 & 0 & 0 & 0 & d_{31} & -d_{22} \\
-d_{22} & d_{22} & 0 & d_{31} & 0 & 0 \\
d_{31} & d_{31} & d_{33} & 0 & 0 & 0
\end{pmatrix} \begin{pmatrix}
0 \\
0 \\
E_z^2 \\
0 \\
0 \\
d_{33} E_z^2
\end{pmatrix} = \varepsilon_0 \begin{pmatrix}
0 \\
0 \\
0
\end{pmatrix},
$$

or simply as $P_z(2\omega) = \varepsilon_0 d_{33} E_z(\omega)^2$.

In QPM wave mixing process, the effective $d_{eff}$ will have a QPM reduction factor of $2/\pi$ in the d-tensor along the selected crystal orientation, i.e. $d_{eff} = \frac{2}{\pi} d$. 