Pryor et al., J. Appl.Phys., Vol. 83, No. 5, 1 March, 1998

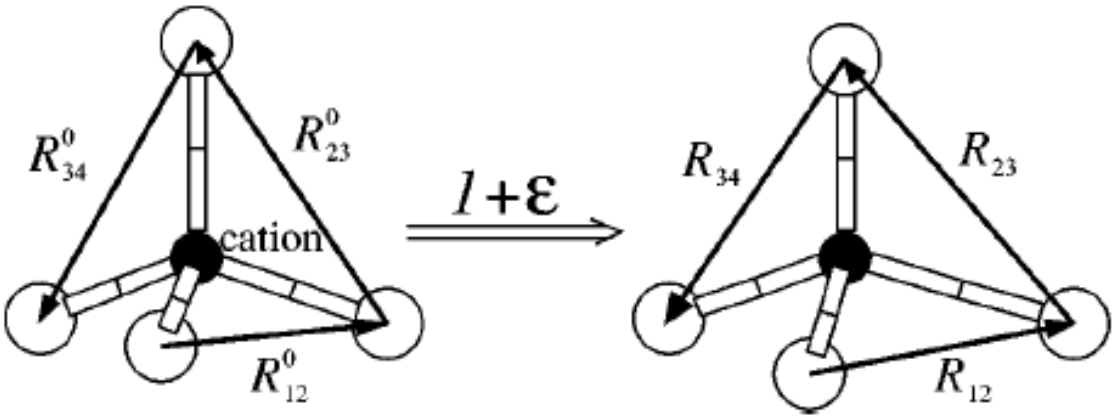

FIG. 2. Schematics to illustrate how the local strain is calculated. For a cation (Ga or In), three vectors ($\{\mathbf{R}\}$) forming a distorted tetrahedron after atomic relaxation are related to the equivalent vectors ($\{\mathbf{R}^0\}$) of an ideal tetrahedron via the strain tensor.

The local strain field is calculated with the relation:

$$\begin{pmatrix} \epsilon_{xx} & \epsilon_{yx} & \epsilon_{zx} \\ \epsilon_{xy} & \epsilon_{yy} & \epsilon_{zy} \\ \epsilon_{xz} & \epsilon_{yz} & \epsilon_{zz} \end{pmatrix} = \begin{pmatrix} R_{12,x} & R_{23,x} & R_{34,x} \\ R_{12,y} & R_{23,y} & R_{34,y} \\ R_{12,z} & R_{23,z} & R_{34,z} \end{pmatrix} \times \begin{pmatrix} R^0_{12,x} & R^0_{23,x} & R^0_{34,x} \\ R^0_{12,y} & R^0_{23,y} & R^0_{34,y} \\ R^0_{12,z} & R^0_{23,z} & R^0_{34,z} \end{pmatrix}^{-1} - I, \tag{19}$$

where I is the unit matrix.