Evaluation of Hydrostatic Component of Strain Tensor from Energy Scan Data Gathered from 34 ID-E

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The decomposition of the full strain tensor into its deviatoric and hydrostatic components can be written as follows.

$$\varepsilon_{Full} = \begin{pmatrix} \varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\ \varepsilon_{21} & \varepsilon_{22} & \varepsilon_{23} \\ \varepsilon_{31} & \varepsilon_{32} & \varepsilon_{33} \end{pmatrix} + \begin{pmatrix} \varepsilon_{hydro} & 0 & 0 \\ 0 & \varepsilon_{hydro} & 0 \\ 0 & 0 & \varepsilon_{hydro} \end{pmatrix} \tag{1}$$

Where $\varepsilon_{hydro}$is the hydrostatic component of the full strain tensor

We can then express the full lattice distortion as a function of ε_{hydro} as follows

$$D(\varepsilon_{hydro}) = \mathrm{I} + \varepsilon_{Full} = \begin{pmatrix} 1+\varepsilon_{11}+\varepsilon_{hydro} & \varepsilon_{12} & \varepsilon_{13} \\ \varepsilon_{21} & 1+\varepsilon_{22}+\varepsilon_{hydro} & \varepsilon_{23} \\ \varepsilon_{31} & \varepsilon_{32} & 1+\varepsilon_{33}+\varepsilon_{hydro} \end{pmatrix} \tag{2}$$

The lattice distortion tensor *D(*ε_{hydro}*)* can now be used to evaluate the real space lattice vector in strained condition using the following relationship.

$$\overrightarrow{R_{Strained}} = D(\varepsilon_{hydro}) \cdot \overrightarrow{R_0} \tag{3}$$

Equivalently, we can write (3) in terms of reciprocal lattice vectors as follows

$$\overrightarrow{Q_{Strained}(h,k,l)} = D(\varepsilon_{hydro})^{-1} \cdot \overrightarrow{Q_0(h,k,l)} \tag{4}$$

For a set of reciprocal lattice vectors $\vec{a^\star}$, $\vec{b^\star}$ and $\vec{c^\star}$ the magnitude of the Q-vector is given as follows.

$$\left\|\vec{Q}\right\| = \left\|h\cdot\vec{a^\star} + k\cdot\vec{b^\star} + l\cdot\vec{c^\star}\right\| \tag{5}$$

The Energy Wire scan measures the magnitude of the Q-vector. Therefore from equation(5) we can write

$$Q_{measured} = \|Q_{Strained}(h,k,l)\| = \left\|D(\varepsilon_{hydro})^{-1} \cdot Q_0(h,k,l)\right\| \tag{6}$$

The objective function can then be expressed as follows

$$\left|Q_{measured} - \left\|D(\varepsilon_{hydro})^{-1} \cdot Q_0(h,k,l)\right\|\right| = Tol \tag{7}$$

The above equation is a function of a single scalar ε_{hydro}. The variable Tol is the specified tolerance.

If we consider a continuous interval where a solution satisfying the objective function would exist , for example [-0.02,0.02] the hydrostatic component can be estimated using an optimization algorithm.

In the FullTensor module we use the Brent Optimization scheme available under SciPy.