# Multislice Diffraction Theory

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#### 1 Functions

#### 1.1 lambda\_from\_eV

This function takes an energy in eV and returns the relativistic electron wavelength. The equation is shown below:

$$\lambda = \sqrt{\frac{h^2 c^2}{E^2 - m_0^2 c^2}} \tag{1}$$

#### 1.2 rotate\_vec\_array

Iterates over each vector in the n x 3 array  $\Lambda$  and rotates them around  $\hat{x}$ ,  $\hat{y}$ , then  $\hat{z}$  by tx, ty, and tz (rad) respectively. That is,

$$\left(\forall v \in \Lambda\right) \left(v \to R_z(\theta_z) \cdot R_y(\theta_y) \cdot R_x(\theta_x) \cdot v = \mathcal{R}v\right) \tag{2}$$

**rotation\_mat** Returns a matrix corresponding to a rotation around  $\hat{x}$ ,  $\hat{y}$ , then  $\hat{z}$  by tx, ty, and tz (rad) respectively.<sup>1</sup>

That is,

$$\mathcal{R} = R_z(\theta_z) \cdot R_y(\theta_y) \cdot R_x(\theta_x) \tag{3}$$

rotation\_mat\_x Returns the rotation matrix around  $\hat{x}$  by  $\theta_x$ ,  $R_x(\theta_x)$ .

**rotation\_mat\_y** Returns the rotation matrix around  $\hat{y}$  by  $\theta_y$ ,  $R_y(\theta_y)$ .

**rotation\_mat\_z** Returns the rotation matrix around  $\hat{z}$  by  $\theta_z$ ,  $R_z(\theta_z)$ .

<sup>&</sup>lt;sup>1</sup>See rotation matrices.