# Novel procedure to construct the displacement matrix of the atoms with thermal vibrations in a face-centered cubic crystal

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**Abstract**

The potential energy $\Phi$ of a crystal can be expanded in a Taylor series of the atomic displacements about their equilibrium positions $\vec{u}^{\,a}_{\ell\kappa} = 0$, where $\ell$ is the unit cell index and $\kappa$ is an atom in that unit cell. Orthogonal directions are indexed by $a$, $b$, and $c$, so:

$$\Phi = \Phi_0 + \sum_{a\ell\kappa} \Phi^a_{\ell\kappa} u^a_{\ell\kappa} + \frac{1}{2} \sum_{a\ell\kappa} \sum_{b\ell'\kappa'} \Phi^{ab}_{\ell\kappa\ell'\kappa'} u^a_{\ell\kappa} u^b_{\ell'\kappa'} + \dots \quad , \tag{1}$$

The second order term of Eq. 1 contains the displacements from equilibrium of pairs of atoms, and the coefficients can be accommodated in $\hat{\Phi}$, the $3 \times 3$ matrix of force constants for those pairs of atoms. The structure of $\hat{\Phi}$ depends of the symmetry of the crystal. The force constants depend on the physics of the interatomic interactions, and in the current application we extracted them from molecular dynamics simulations. In this talk, we will describe how we build a displacement matrix $\hat{\mathcal{U}}$ that minimizes the number of unknowns and hence the computational cost of computing the lattice dynamics.

We exploit the symmetries of the crystal and introduce two auxiliary matrices which separate the diagonal and off-diagonal components of the displacements:

$$m_1 = \begin{pmatrix} U_{nx} & 0 & 0 \\ 0 & U_{ny} & 0 \\ 0 & 0 & U_{nz} \end{pmatrix} \tag{2}$$

and

$$m_2 = \begin{pmatrix} 0 & U_{ny} & U_{nz} \\ U_{nx} & 0 & U_{nz} \\ U_{nx} & U_y & 0 \end{pmatrix} \quad \text{with } n \text{ as time step.} \tag{3}$$

We define matrix operations involving $m_1$ and $m_2$ for each of the five nearest neighbors to populate $\hat{\mathcal{U}}$, which has number of force constants (FC) rows and three times the number of atoms (3N) columns. The matrix multiplication of the pseudo-inverse of $\hat{\mathcal{U}}$ times the forces acting on each orthogonal direction of each atom obtained from the physics simulations is the vector of force constants $\hat{\mathcal{P}}$. Finally, the dynamical matrix $\hat{\mathcal{D}}$, from which the lattice dynamics of the system are extracted, is obtained by taking the Fourier transforms of appropriate force constant matrices built using the elements of $\hat{\mathcal{P}}$. We will show results for face-centered cubic nickel.