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Cross Lattice and Eigenfunctions

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Reciprocal lattice is, widely, used in the theory of solids. The reciprocal lattice vectors have dimensions of inverse of length. These vectors are, therefore, different in different systems of units. Cross lattice was defined in such a way that the cross-lattice vectors were independent of the coördinate system chosen. A coördinate-independent representation is a pre-requisite of representing generalized laws and forms the basis of principle of general covariance. Let $\hat{\boldsymbol{a}}_1$, $\hat{\boldsymbol{a}}_2$, $\hat{\boldsymbol{a}}_3$, be the basis vectors for ordinarty lattice. Any vector $\boldsymbol{L}$, was be represented in terms of these linearly-independent bases $\boldsymbol{L} = L_k\, \hat{\boldsymbol{a}}_k$ (repeated indices denote summation according to Einstein convention; all latin indices take up the values 1, 2, 3). The recipriocal-latttice vectors for a non-rectangular lattice, were constructed, using the basis vectors ($\in_{klm}$ is Levi-Civita symbol)

$$\hat{\boldsymbol{g}}_k = \in_{klm} \frac{\hat{\boldsymbol{a}}_l \times \hat{\boldsymbol{a}}_m}{2\hat{\boldsymbol{a}}_1 \bullet \hat{\boldsymbol{a}}_2 \times \hat{\boldsymbol{a}}_3}$$

as $\boldsymbol{G} = G_k\, \hat{\boldsymbol{g}}_k = 2\pi\, n_k\, \hat{\boldsymbol{g}}_k$; the numbers n_k were integers, this condition was obtained by applying the periodicity condition $f(r+L) = f(r)$. The reciprocal lattice vectors satisfied the condition $\hat{\boldsymbol{a}}_i \bullet \hat{\boldsymbol{g}}_j = \delta_{ij}$; where δ_{ij} is Knoecker delta. A cross product of the direct- and the rciprocal-lattice vectors was dimensioneless, and named as *cross lartice*, $\hat{\boldsymbol{e}}_i = \hat{\boldsymbol{a}}_i \times \hat{\boldsymbol{g}}_i$ (no summation over i). The cross-lattice length was written as $\boldsymbol{D} = D_k\, \hat{\boldsymbol{e}}_k = 2\pi\, n_k\, \hat{\boldsymbol{e}}_k$. The following results were derived from the above deinition, $\boldsymbol{D} \bullet \boldsymbol{L} = \boldsymbol{D} \bullet \boldsymbol{G} = 0$; $\exp(i\boldsymbol{D} \bullet \boldsymbol{L}) = \exp(i\boldsymbol{D} \bullet \boldsymbol{G}) = 1$ ($i = \sqrt{-1}$). The eigenfunctions of cross lattice were obtained by considring an anisotropic potential, which depended on angle, θ. The band must be well separated so that the non-diagonal matrix elements vanished with respect to band index. Defining a modified Brillouin zone to a Wigner-Seitz cell in cross lattice, and letting $\boldsymbol{D}$ take all values inside this zone, all the coefficients varied and became functions of $\boldsymbol{D}$. However, because of the periodicity in the momentum space, they were all identical functions of $\boldsymbol{D}$, translated in cross-lattice space. Wannier functions (Fig. 1) are useful for systems, which are *isotroptic*, but *inhomogeneous*. The cross eigenfunctions, belonging to eigen-states of angular momentum in cross-lattice representation, are useful for systems, which are *homogeneous*, but *anisotropic*[§].

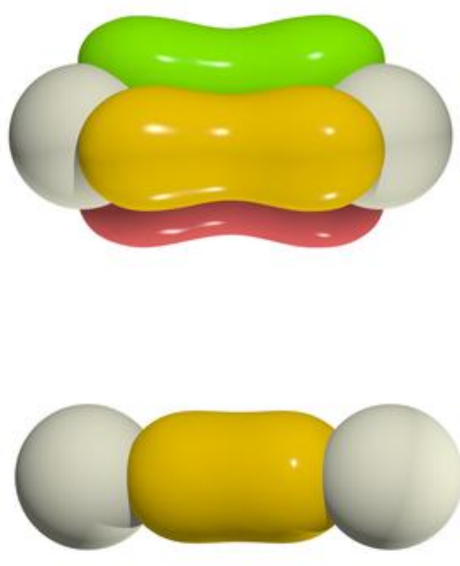

Fig. 1. Wannier functions of triple- and single-bonded nitrogen dimmers in palladium nitride

Keywords: Crystal structure • Momentum eigenfunctions • Reciprocal lattice • Wannier functions

Web address of this document: https://www.ngds-ku.org/Presentations/Cross.pdf

[§]A decade later these results have been published in a peer-reviewed journal — Kamal, S. A. and S. A. Husian (1988). A dimensionless reciprocal lattice. *Karachi University Journal of Science*, **16 (1&2):** 23-27, full text: https://www.ngds-ku.org/Papers/J07.pdf