# Chapter 1: Reciprocal Lattice, Covariant and Contravariant Tensors

## 1.1. Review of the Reciprocal Lattice

Dear students, today we will delve into a fundamental concept in materials science: the reciprocal lattice. We will begin by reviewing its definition and properties, then explore the crucial concepts of covariant and contravariant tensors, and finally understand how these ideas relate to the real and reciprocal lattices.

The reciprocal lattice is an indispensable tool in understanding phenomena such as X-ray diffraction, electron diffraction, and the electronic band structure of solids. It provides a convenient framework for visualizing and calculating wave-particle interactions within periodic structures.

### 1.1.1. Definition and Fundamental Properties

The reciprocal lattice is defined in terms of the basis vectors of the real-space lattice. Let the primitive basis vectors of the real-space lattice be $ \_1, \_2, \_3

$$. The corresponding primitive basis vectors of the reciprocal lattice, denoted as $ \mathbf{a}^\*\_1, \mathbf{a}^\*\_2, \mathbf{a}^\*\_3 $$

, are defined such that they satisfy the following orthonormalization condition:

Here, $ \_{ij}

$$ is the Kronecker delta, which is 1 if $ i=j $$

and 0 if $ i j

$$. The factor of $ 2\pi $$

is a convention often used in physics, particularly in solid-state physics and Fourier transforms, to simplify later equations (e.g., Bragg’s law). Some crystallography texts may omit the $ 2

$$, defining $ \mathbf{a}^\*\_i \cdot \mathbf{a}\_j = \delta\_{ij} $$

. It is important to be aware of the convention used in any given text or problem.

From this definition, we can explicitly derive the reciprocal lattice basis vectors. By performing the dot product operations and solving the system of equations, we find:

where $ V $$ is the volume of the real-space primitive unit cell, given by the scalar triple product:

**Key properties resulting from this definition include:**

* **Orthogonality:** Each reciprocal lattice vector $ ^\*\_i

$$ is perpendicular to the two real-space basis vectors that are \*not\* $ \mathbf{a}\_i $$

* . For example, $ ^\*\_1

$$ is perpendicular to both $ \mathbf{a}\_2 $$

* and $ \_3 $$. This is evident from the cross-product definition.
* **Magnitude:** The magnitude of a reciprocal lattice vector is inversely proportional to the spacing between the set of real-space lattice planes to which it is normal. For example, in a simple orthogonal system, $ |^\*\_1| = 2/|\_1|

$$. More generally, $ |\mathbf{a}^\*\_1| $$

* is inversely proportional to the interplanar spacing of the lattice planes defined by $ \_2

$$ and $ \mathbf{a}\_3 $$

* .

### 1.1.2. Graphical Construction of the Reciprocal Lattice

While the mathematical definition is precise, it’s also helpful to visualize the reciprocal lattice, especially for 2D systems. Let’s consider a 2D real-space lattice defined by primitive vectors $ \_1

$$ and $ \mathbf{a}\_2 $$

.

1. **Orientation:** The reciprocal vector $ ^\*\_1

$$ is perpendicular to $ \mathbf{a}\_2 $$

* , and $ ^\*\_2

$$ is perpendicular to $ \mathbf{a}\_1 $$

* . We can start by drawing $ ^\*\_1

$$ perpendicular to $ \mathbf{a}\_2 $$

* and $ ^\*\_2

$$ perpendicular to $ \mathbf{a}\_1 $$

* .

1. **Length:** The lengths of the reciprocal basis vectors are inversely related to the lengths of the real-space basis vectors. Roughly, $ |^\*\_1| /|\_1|

$$ and $ |\mathbf{a}^\*\_2| \propto 1/|\mathbf{a}\_2| $$

* .

1. **Angle:** The angle between $ ^\*\_1

$$ and $ \mathbf{a}^\*\_2 $$

* in the reciprocal lattice is the supplement (i.e., $ 180^-

$$) of the angle between $ \mathbf{a}\_1 $$

* and $ \_2

$$ in the real lattice, where $ \theta $$

* is the angle between $ \_1

$$ and $ \mathbf{a}\_2 $$

* .

**Important Note:** These simple graphical rules (especially concerning proportionality of lengths and angle relations) are exactly true only for orthogonal coordinate systems (e.g., cubic, tetragonal, orthorhombic with $ ==^$$). For general oblique systems, such as monoclinic or triclinic lattices, these relationships hold approximately but are not strictly accurate. However, they provide a good qualitative understanding of the reciprocal lattice geometry. For precise constructions, the mathematical definitions must always be used.

**Historical Background:** The concept of the reciprocal lattice was developed by **J. Willard Gibbs** in the late 19th century as a mathematical tool for crystallography and vector analysis. Its physical significance became profoundly clear with the discovery of X-ray diffraction by **Max von Laue** in 1912 and the subsequent formulation of **Bragg’s Law** by **William Henry Bragg** and **William Lawrence Bragg** in 1913. These discoveries showed that the diffraction patterns from crystals could be elegantly interpreted as a direct mapping of the crystal’s reciprocal lattice.

### 1.1.3. Constructing Reciprocal Lattice Points and the Uniqueness Issue

Once we have established the reciprocal lattice primitive basis vectors, we can construct the entire reciprocal lattice by taking integer linear combinations of these vectors. A general reciprocal lattice vector $ $$ is given by:

where $ h, k, l

$$ are integers, commonly known as Miller indices in real space. These integers now represent the coordinates of a reciprocal lattice point. Each point $ (hkl) $$

in reciprocal space corresponds to a family of parallel lattice planes in real space.

Let’s illustrate this with an example. Consider a 2D real-space Bravais lattice. If we select specific primitive basis vectors for this Bravais lattice, say $ \_A

$$ and $ \mathbf{a}\_B $$

, we can derive the corresponding reciprocal lattice vectors $ ^\*\_A

$$ and $ \mathbf{a}^\*\_B $$

. The reciprocal lattice points will then be formed by combining these vectors.

However, a critical point arises: the choice of primitive unit cell in real space is not unique for a given lattice. As we discussed earlier, for a given set of lattice points, one can draw multiple primitive unit cells. Each choice of real-space primitive vectors will lead to a different set of reciprocal lattice vectors.

For instance, if we start with one set of real-space primitive vectors (e.g., $ \_1, \_2

$$), we generate one reciprocal lattice. If we choose a different set of real-space primitive vectors (e.g., $ \mathbf{a}'\_1, \mathbf{a}'\_2 $$

) for the *same* real-space lattice, we will generate a *different* set of primitive reciprocal lattice vectors. This might lead to an apparent difference in the arrangement of reciprocal lattice points if we only consider the *primitive* sets.

This non-uniqueness might seem problematic. If the reciprocal lattice depends on our arbitrary choice of real-space primitive vectors, how can it represent a fundamental property of the crystal? The key insight is that **the reciprocal lattice must be constructed from the *lattice points* of the real lattice, not from an arbitrarily chosen unit cell or basis vectors.**

In other words, the reciprocal lattice is fundamentally determined by the *set of all real-space lattice points* and their periodicity, not by a specific set of primitive vectors used to *describe* that periodicity. This means that while different sets of primitive vectors for the *same* lattice will generate different *primitive* reciprocal lattice vectors, the *entire set of reciprocal lattice points* should be consistent and reflect the underlying periodicity of the real lattice. The apparent “problem” of non-uniqueness will be fully resolved once we account for the crystal’s internal symmetries through extinction rules, which we will discuss next.

## 1.2. Physical Significance: The Reciprocal Lattice as a Fourier Transform

To truly grasp the essence of the reciprocal lattice, it is crucial to understand its profound connection to the **Fourier transform**.

The reciprocal lattice is precisely the set of wave vectors $

$$ for which a plane wave $ e^{i \mathbf{G} \cdot \mathbf{r}} $$

has the same periodicity as the real-space lattice. Mathematically, the reciprocal lattice points are the wave vectors in Fourier space that correspond to the periodicity of the crystal structure.

This concept is paramount in fields like: \* **X-ray Diffraction (XRD):** The diffraction pattern observed from a crystal is essentially a map of its reciprocal lattice. The peaks in the diffraction pattern correspond directly to the reciprocal lattice points. The positions of these peaks reveal the dimensions and symmetry of the reciprocal lattice, which in turn tells us about the real-space crystal structure. \* **Solid-State Physics:** In band theory, the electronic energy bands of a crystal are typically plotted in reciprocal space, particularly within the **Brillouin zone**, which is a primitive unit cell of the reciprocal lattice. This is because the Bloch wave functions describing electrons in a periodic potential are characterized by wave vectors in reciprocal space. The Brillouin zone is the fundamental domain for describing electron momentum in a crystal.

Both X-ray diffraction and solid-state band theory fundamentally rely on understanding the **interference** of waves—whether electromagnetic waves (X-rays) or matter waves (electrons). The reciprocal lattice provides the natural framework for analyzing these interference phenomena.

### 1.2.1. Reciprocal Lattice in Scattering Theory

Let’s revisit the core idea of scattering. When waves (like X-rays or electrons) interact with a material, they are scattered by the electron density distribution or the nuclear spin distribution within the material. The scattered wave amplitude, $ S()

$$, is given by the Fourier transform of this distribution $ \rho(\mathbf{r}) $$

. Here, $

$$ represents the scattering vector, which is the difference between the incident wave vector $ \mathbf{k}\_0 $$

and the scattered wave vector $ ’

$$ (i.e., $ \mathbf{K} = \mathbf{k}' - \mathbf{k}\_0 $$

).

The general scattering amplitude can be expressed as:

For a crystalline material, the electron density $ ()

$$ is periodic, meaning $ \rho(\mathbf{r}) = \rho(\mathbf{r} + \mathbf{R}) $$

for any real-space lattice vector $

$$. Due to this periodicity, the Fourier transform $ S(\mathbf{K}) $$

will only be non-zero for specific values of $

$$. These specific values are precisely the reciprocal lattice vectors $ \mathbf{G} $$

. This implies that a diffraction peak (or strong scattering) will only occur if the scattering vector $

$$ coincides with a reciprocal lattice vector $ \mathbf{G} $$

. This condition, $ = $$, is known as the **Laue condition**.

The Laue condition is entirely equivalent to **Bragg’s Law**. Bragg’s Law states that for constructive interference to occur (i.e., for a diffraction peak to be observed), the path difference between waves scattered from adjacent atomic planes must be an integer multiple of the wavelength. Mathematically, this is expressed as:

where $ d

$$ is the interplanar spacing, $ \theta $$

is the Bragg angle, $ n

$$ is an integer, and $ \lambda $$

is the wavelength. In reciprocal space, the magnitude of a reciprocal lattice vector $ *{hkl} $$ is $ |\mathbf{G}\_{hkl}| = 2\pi/d\_{hkl} $$ (using the $ 2$$ convention). The Bragg condition in reciprocal space is then $ |\mathbf{K}| = |\mathbf{G}\_{hkl}| $$ and $ $$ is parallel to $ \mathbf{G}\_{hkl} $$. The combination of these results in $ =* {hkl} $$.

From this, it becomes clear that in the reciprocal lattice, only those points corresponding to a non-zero scattering amplitude $ S() $$ have physical significance. These are the points where constructive interference occurs, leading to observable diffraction spots.

### 1.2.2. Extinction Rules and Bravais Lattice Transformations

The discussion about the non-uniqueness of reciprocal lattice basis vectors, which led to different reciprocal lattice point arrangements, needs to be addressed. This apparent contradiction is resolved by considering **extinction rules (or selection rules)** in diffraction.

Extinction rules arise from the internal structure of the unit cell, specifically the presence of centering atoms (e.g., in face-centered cubic, body-centered cubic, or base-centered lattices) or certain symmetry elements like screw axes and glide planes. These additional symmetries lead to destructive interference for certain Bragg reflections, effectively “extinguishing” specific reciprocal lattice points. In essence, while a particular set of Miller indices $ (hkl)

$$ might correspond to a potential reciprocal lattice point, if the structure factor $ F\_{hkl} $$

for that point is zero due to symmetry, no diffraction will be observed, and that point is “extinguished.”

When plotting the reciprocal lattice, we must take these extinction rules into account. The points that are “extinguished” (i.e., for which the structure factor $ F\_{hkl} $$ is zero) should be removed from the reciprocal lattice plot.

Let’s reconsider the example from earlier. If we have a face-centered cubic (FCC) Bravais lattice in real space, its primitive basis vectors will lead to one reciprocal lattice. However, the extinction rules for an FCC lattice state that reflections are present only if $ h, k, l

$$ are all even or all odd (i.e., $ h+k+l = \text{even} $$

for *all allowed* reflections, not odd). If we apply these rules and remove the “extinguished” points, the resulting set of *allowed* reciprocal lattice points forms a body-centered cubic (BCC) lattice.

This means that while the initial primitive reciprocal lattice vectors might differ based on the choice of real-space primitive vectors, applying the correct extinction rules ensures that the *physically relevant* reciprocal lattice points form a unique and consistent reciprocal Bravais lattice. This resolves the ambiguity and confirms that the reciprocal lattice is indeed a fundamental property of the crystal structure.

**Example for an FCC real-space lattice:** The condition for reflection from an FCC lattice is that $ h, k, l $$ must be either all even or all odd. Reflections with mixed parity (e.g., one even, two odd) are extinguished. If we remove these extinguished points, the remaining points form a body-centered cubic (BCC) lattice in reciprocal space.

This correspondence between real-space Bravais lattices and their reciprocal counterparts is a powerful consequence of crystallography and Fourier analysis.

### 1.2.3. Correspondence Between Real and Reciprocal Bravais Lattices

Let’s summarize the fascinating relationships between real-space Bravais lattices and their reciprocal space counterparts, taking into account extinction rules.

| Real-Space Bravais Lattice Type | Extinction Rule for $ (hkl) $ Reflections | Reciprocal Bravais Lattice Type |
| --- | --- | --- |
| Simple Cubic (SC) | All $ h, k, l  $$ allowed | Simple Cubic (SC) | | Body-Centered Cubic (BCC) | $ h+k+l = \text{even} $$  (e.g., (110), (200)) | Face-Centered Cubic (FCC) |
| Face-Centered Cubic (FCC) | $ h, k, l  $$ all even or all odd (e.g., (111), (200), (220)) | Body-Centered Cubic (BCC) | | Simple Hexagonal (SH) | All $ h, k, l $$  allowed | Simple Hexagonal (SH) |
| Primitive Triclinic (P) | All $ h, k, l  $$ allowed | Primitive Triclinic (P) | | Primitive Monoclinic (P) | All $ h, k, l $$  allowed | Primitive Monoclinic (P) |
| Base-Centered Monoclinic (C) | $ h+k =  $$ | Primitive Monoclinic (P) | | Primitive Orthorhombic (P) | All $ h, k, l $$  allowed | Primitive Orthorhombic (P) |
| Base-Centered Orthorhombic (C) | $ h+k =  $$ | Face-Centered Orthorhombic (F) | | Body-Centered Orthorhombic (I) | $ h+k+l = \text{even} $$ | Base-Centered Orthorhombic (C) |
| Face-Centered Orthorhombic (F) | $ h, k, l  $$ all even or all odd | Body-Centered Orthorhombic (I) | | Primitive Tetragonal (P) | All $ h, k, l $$  allowed | Primitive Tetragonal (P) |
| Body-Centered Tetragonal (I) | $ h+k+l =  $$ | Face-Centered Tetragonal (F) | | Rhombohedral (R) | All $ h, k, l $$  allowed | Rhombohedral (R) |

**Key Observations:** \* Simple lattices remain simple in reciprocal space. \* BCC transforms to FCC, and FCC transforms to BCC. This duality is a beautiful consequence of their specific centering and the resulting destructive interference patterns. \* Body-centered transforms to face-centered, and vice versa, for various other crystal systems as well.

This table highlights how the specific symmetries and centering of a real-space Bravais lattice uniquely determine the type of Bravais lattice in reciprocal space. This is why the reciprocal lattice is such a powerful tool for analyzing crystal structures from diffraction experiments.

**Practical Application:** Visualizing these lattices and their reciprocal counterparts is an excellent way to solidify your understanding. A program like crystaldrawcell.py (which might be a custom script or a similar educational tool) that draws reciprocal unit cells (often highlighted with red lines) can be very instructive. By examining its code, you can learn the algorithms for calculating and visualizing reciprocal lattices, which is a valuable skill in computational materials science.

## 1.3. Introduction to Covariant and Contravariant Vectors

To fully comprehend the intricate relationship between the real lattice and the reciprocal lattice, we must introduce the concepts of **covariant and contravariant vectors**. These are fundamental in tensor calculus and provide a rigorous framework for understanding how physical quantities transform under coordinate changes.

### 1.3.1. Lattice Transformation Rules Revisited

Let’s recall the rules for lattice transformations that we discussed in a previous lecture. When we change our coordinate system (e.g., choose a different set of basis vectors), how do our physical quantities transform?

Suppose we have an old set of real-space primitive basis vectors $ { \_j }

$$ and a new set $ \{ \mathbf{a}'\_i \} $$

. The transformation between them can be described by a transformation matrix $ $$.

1. **Transformation of Real-Space Basis Vectors:** The new basis vectors are linear combinations of the old ones:

* (Here, $ T\_{ij}

$$ are the components of the transformation matrix $ \mathbf{T} $$

* . The summation is over the old basis vectors $ \_j $$.)

1. **Transformation of Real-Space Coordinates:** If a real-space vector $

$$ is expressed as $ \mathbf{r} = \sum\_j x^j \mathbf{a}\_j $$

* , then its coordinates $ x^j

$$ transform under the inverse transpose of the matrix $ \mathbf{T} $$

* .
* This can also be written as $ x’^i = *j (T{-1})T*{ij} x^j

$$, where $ (T^{-1})^T $$

* denotes the transpose of the inverse matrix.

1. **Transformation of Reciprocal-Space Basis Vectors:** The reciprocal basis vectors $ ^\*\_i

$$ transform under the inverse transpose of $ \mathbf{T} $$

* .

1. **Transformation of Reciprocal-Space Coordinates (Miller Indices):** The coordinates in reciprocal space (Miller indices $ h, k, l

$$) transform directly with the matrix $ \mathbf{T} $$

* .

(Note: In this initial review, the indices are not yet following the strict Einstein convention of upper/lower for contravariant/covariant. This will be introduced shortly.)

### 1.3.2. Defining Covariant and Contravariant Vectors

Observing these transformation rules, we can categorize vectors (and their components) into two distinct types:

1. **Covariant Vectors (or Vectors that “Co-vary”):** These are quantities whose components transform in the *same way* as the basis vectors themselves. In our lattice transformation example, real-space basis vectors $ \_j

$$ and reciprocal-space coordinates (Miller indices $ h^j $$

* ) belong to this group. Their components transform directly with the transformation matrix $ $$.
  + **Co-variant** literally means “transforming together” or “in the same way” as the basis vectors.
  + Think of them as quantities that, when paired with appropriate components, lead to an invariant physical vector.

1. **Contravariant Vectors (or Vectors that “Contra-vary”):** These are quantities whose components transform in the *inverse transpose* manner relative to the basis vectors. In our example, real-space coordinates $ x^j

$$ and reciprocal-space basis vectors $ \mathbf{a}^\*\_j $$

* fall into this category. Their components transform with the inverse of the transformation matrix that transforms the basis vectors.
  + **Contra-variant** means “transforming oppositely” or “in the inverse way” compared to the basis vectors.
  + These are usually the “coordinates” or “components” that project onto the basis vectors.

This distinction is crucial because it ensures that physical quantities, which are inherently independent of the chosen coordinate system, remain invariant under transformations. The components change in a specific way to compensate for the change in the basis vectors.

**Historical Context:** The concepts of covariance and contravariance were formalized within tensor calculus, which gained prominence with **Albert Einstein’s theory of general relativity** in the early 20th century. Einstein realized that to formulate physical laws that held true in all coordinate systems (including accelerating and curved ones), these laws needed to be expressed in a “covariant” form, meaning the equations themselves maintained their structure under general coordinate transformations. This led to the widespread use of tensor notation and the distinction between covariant and contravariant components.

## 1.4. Metric Tensor and its Transformation Properties

The **metric tensor** is a fundamental quantity that allows us to measure lengths, angles, and volumes in a given coordinate system. It essentially encodes the geometry of the space.

### 1.4.1. Definition of the Metric Tensor in Real Space

For the real-space lattice, the metric tensor $ g\_{ij} $$ is defined by the dot product of the real-space basis vectors:

This definition allows us to calculate the squared length of any vector $ = x^i \_i $$. Let’s explicitly show this derivation:

Substitute $ = x^i \_i

$$ and $ \mathbf{r} = x^j \mathbf{a}\_j $$

. (We use a different index $ j

||^2 = (x^i \_i) (x^j \_j)

||^2 = x^i x^j (\_i *j) ||^2 = x^i x^j g*{ij} $$

The metric tensor $ g\_{ij}

$$ is symmetric, meaning $ g\_{ij} = g\_{ji} $$

.

### 1.4.2. Transformation of the Real-Space Metric Tensor

Let’s examine how the real-space metric tensor transforms under a change of basis. If $ ’\_i = *k T*{ik} \_k

$$ are the new basis vectors, then the new metric tensor $ g'\_{ij} $$

is:

Substitute the transformation rule for $ ’*i $$ and $ \mathbf{a}'\_j $$. Since the dot product is linear and commutative, we can rearrange the sums and the dot product: Recognizing $ k l = g{kl} g’{ij} = k l T{ik} T{jl} g*{kl} $$

This transformation rule shows that the components of $ g\_{ij}

$$ transform with \*two\* factors of the transformation matrix $ \mathbf{T} $$

. This indicates that $ g\_{ij} $$ is a **second-rank covariant tensor** (or a 2-times covariant tensor). It “co-varies” with respect to both indices.

### 1.4.3. Definition and Transformation of the Reciprocal-Space Metric Tensor

Similarly, we can define a metric tensor for the reciprocal space, often denoted as $ g^{ij} $$ (with upper indices to denote its contravariant nature, as we will formalize soon):

This tensor allows us to calculate the squared length of a reciprocal lattice vector $ = h\_i ^\*\_i $$ (using covariant indices for reciprocal space components). Let’s derive this:

Substitute $ = h\_i ^\*\_i

$$ and $ \mathbf{G} = h\_j \mathbf{a}^\*\_j $$

.

Now, let’s consider its transformation. The reciprocal basis vectors $ ^\*\_i

$$ transform contravariantly. If $ \mathbf{a}'^\*\_i = \sum\_k (T^{-1})\_{ki} \mathbf{a}^\*\_k $$

, then the new reciprocal metric tensor $ g’^{ij} $$ is:

This transformation rule indicates that $ g^{ij}

$$ transforms with \*two\* factors of the inverse transpose of the transformation matrix $ \mathbf{T} $$

. This makes $ g^{ij} $$ a **second-rank contravariant tensor** (or a 2-times contravariant tensor).

**Relationship between $ g\_{ij} $$ and $ g^{ij} $$.** A crucial relationship exists between the real-space and reciprocal-space metric tensors: they are matrix inverses of each other (up to a scalar factor depending on the $ 2

*k g*{ik} g^{kj} = \_i^j

$$
This means that if we represent $ g\_{ij} $$

as a matrix $

$$, and $ g^{ij} $$

as a matrix $ ^\*

$$, then $ \mathbf{G}^\* = \mathbf{G}^{-1} $$

. This elegantly links the geometry of real space to that of reciprocal space.

Understanding the transformation properties of the metric tensor is vital as it governs how magnitudes and angles are perceived in different coordinate systems. It also serves as a prototype for identifying the covariant or contravariant nature of other tensors in materials science.

## 1.5. Relation Between Real-Space and Reciprocal-Space Transformations

Let’s delve deeper into how the real and reciprocal lattice basis vectors are mathematically connected through transformation matrices, building upon the metric tensor concept.

Recall the defining relationship between real and reciprocal primitive basis vectors:

This equation is a powerful statement. If we form a matrix where the $ i $-th row contains the components of $ ^\*\_i

$$ and a matrix where the $ j $-th column contains the components of $ \mathbf{a}\_j $$

, then the matrix product of these (effectively, dot products of row vectors from one set with column vectors from the other) yields a diagonal matrix, specifically $ 2$$ times the identity matrix.

Let’s represent the real-space basis vectors as rows of a matrix $

$$ and reciprocal-space basis vectors as rows of a matrix $ \mathbf{A}^\* $$

. Then, the defining relationship implies:

where $ $$ is the identity matrix. From this, we can deduce the direct relationship between the basis vectors’ component matrices:

or

This shows that the matrix of reciprocal basis vectors is directly related to the inverse transpose of the matrix of real-space basis vectors. This is consistent with the contravariant transformation property we observed for reciprocal basis vectors.

Now, let’s consider the components of a general vector $

= X^i \_i = H\_i ^\*\_i

$$
Here $ X^i $$

are contravariant components (real-space coordinates), and $ H\_i $$ are covariant components (reciprocal-space coordinates, i.e., Miller indices).

Let’s take the dot product of $

$$ with a real-space basis vector $ \mathbf{a}\_j $$

.

This shows that $ \_j

$$ yields covariant components. So, $ X\_j = X^i g\_{ij} $$

.

And taking the dot product with a reciprocal-space basis vector $ ^\*\_j

^\*\_j = (H\_i ^\*\_i) ^\*\_j = H\_i (^\*\_i ^\*\_j) = H\_i g^{ij}

$$
This shows that $ \mathbf{R} \cdot \mathbf{a}^\*\_j $$

yields contravariant components. So, $ H^j = H\_i g^{ij} $$.

This implies that the metric tensors act as “converters” between covariant and contravariant components of a vector. Specifically, to convert contravariant components $ X^j

$$ to covariant components $ X\_i $$

:

And to convert covariant components $ X\_j

$$ to contravariant components $ X^i $$

:

This relationship is a direct consequence of the definition of the reciprocal lattice and its close connection to the metric tensors. The transformation rules for real and reciprocal lattice vectors and their coordinates are profoundly linked through these metric tensors, which fundamentally define the geometry of the respective spaces.

In simpler terms, if you have a set of real-space basis vectors, you can compute the real-space metric tensor. The inverse of this metric tensor (scaled by a factor of $ (2)^2 $$ depending on conventions) effectively gives you the metric tensor of the reciprocal space. This inverse relationship highlights the duality between real and reciprocal space.

## 1.6. Invariance of Scalar Products

One of the most powerful aspects of distinguishing between covariant and contravariant vectors is the guarantee that their dot product (or scalar product) is always an invariant quantity, meaning it does not change under coordinate transformations. This is a fundamental requirement for any physical law, as physical quantities themselves should not depend on our choice of coordinate system.

Let’s consider a physical vector $ $$. We can express this vector using either contravariant components and covariant basis vectors, or covariant components and contravariant basis vectors. For example:

where $ x^i

$$ are the contravariant components and $ \mathbf{a}\_i $$

are the covariant basis vectors.

Now, consider a scalar product between two vectors, say $

$$ and $ \mathbf{B} $$

. Let’s express $

$$ using its contravariant components $ A^i $$

and covariant basis $ \_i

$$ (i.e., $ \mathbf{A} = A^i \mathbf{a}\_i $$

) and $

$$ using its covariant components $ B\_j $$

and contravariant basis $ ^\*\_j

$$ (i.e., $ \mathbf{B} = B\_j \mathbf{a}^\*\_j $$

).

The dot product $ $$ would be:

From the definition of reciprocal lattice, $ \_i ^\**j = 2*{ij}

= A^i B\_j (2\_{ij})

= 2\_i A^i B\_i $$

The crucial point here is that when one component is contravariant (upper index) and the other is covariant (lower index), and they are contracted (summed over), the result is a scalar invariant. Let’s explicitly verify the invariance of a vector itself under transformations.

Let a vector $

= x^i \_i

= x’^k ’\_k $$

We know the transformation rules:

(Here, for clarity, $ T\_{kj}

$$ means the matrix element in row $ k $ and column $ j $, and $ (T^{-1})\_{lk} $$

means the element in row $ l $ and column $ k $ of the inverse matrix.)

Substituting these into the transformed expression for $ $$, we get:

Rearrange the summation order:

The term in the parenthesis is $ *k (T^{-1})*{lk} T\_{kj}

$$. This is precisely the definition of the matrix product of $ \mathbf{T}^{-1} $$

and $

$$. Since $ \mathbf{T}^{-1}\mathbf{T} = \mathbf{I} $$

(the identity matrix), this sum evaluates to the Kronecker delta $ \_{lj} $$.

So, the equation simplifies to:

The Kronecker delta forces $ l=j

$$, so only terms where $ l=j $$

survive:

This confirms that the vector $ $$ itself is invariant under coordinate transformations, even though its components and basis vectors change. This fundamental property holds for any pair of covariant and contravariant quantities whose indices are contracted.

This fundamental property is why the distinction between covariant and contravariant quantities is so important in physics and engineering. It allows us to formulate laws that hold true regardless of the observer’s coordinate system.

## 1.7. Einstein Summation Convention

To make tensor equations more concise and to immediately identify covariant and contravariant quantities, a specific notation system is widely adopted: the **Einstein Summation Convention**.

### 1.7.1. Rules of the Einstein Summation Convention

The convention, introduced by Albert Einstein, establishes two simple but powerful rules for index placement:

1. **Covariant indices are written as subscripts (lower indices):** These typically denote components that transform like basis vectors or components of a covariant tensor.
   * Example: $ A\_i $$ for a covariant vector component.
   * Example: $ g\_{ij} $$ for the covariant metric tensor.
2. **Contravariant indices are written as superscripts (upper indices):** These typically denote components that transform inversely to basis vectors or components of a contravariant tensor.
   * Example: $ A^i $$ for a contravariant vector component.
   * Example: $ g^{ij} $$ for the contravariant metric tensor.
3. **Implied Summation (Contraction):** If an index appears exactly once as a subscript and exactly once as a superscript in a single term, then summation over that index is implied, and the summation symbol ($ $$) can be omitted. This is called **contraction**.

**Benefits of this Notation:**

* **Conciseness:** Equations become much shorter and easier to read without explicit summation symbols. For example, $ \_i A^i B\_i

$$ becomes $ A^i B\_i $$

* .
* **Clarity on Invariance:** If all indices in an expression are contracted (i.e., every index appears once as a subscript and once as a superscript), the resulting quantity is a scalar invariant. This provides an immediate visual check for the scalar nature of an expression.
* **Consistency Check:** In a valid tensor equation, the free indices (those not summed over) must appear in the same position (upper or lower) on both sides of the equation. This helps prevent errors in tensor manipulation and ensures the equation is covariant.

### 1.7.2. Rewriting Quantities with Einstein Notation

Let’s re-examine the quantities we’ve discussed using the Einstein summation convention:

* **Real-space primitive basis vectors:** These transform directly with the transformation matrix $

$$. Thus, they are covariant. We denote them as $ \mathbf{a}\_i $$

* .
* **Real-space metric tensor:** Defined as $ \_i *j $$, it transforms with two factors of $ \mathbf{T} $$. Thus, it is a second-rank covariant tensor: $ g*{ij} $$.
* **Reciprocal-space coordinates (Miller indices):** These transform directly with $

$$. Thus, they are covariant components: $ h\_i $$

* .
* **Real-space coordinates:** These transform with the inverse transpose of $

$$. Thus, they are contravariant components: $ x^i $$

* . A real-space vector is written as $ = x^i \_i $$.
* **Reciprocal-space primitive basis vectors:** These transform with the inverse transpose of $

$$. Thus, they are contravariant: $ \mathbf{a}^i $$

* . (Note: We use $ ^i

$$ instead of $ \mathbf{a}^\*\_i $$

* when using Einstein notation to implicitly denote its contravariant nature. However, for clarity in specific contexts, $ ^\*\_i $$ is still often used to distinguish from real-space vectors).
* **Reciprocal-space metric tensor:** Defined as $ ^\*\_i ^\*\_j

$$, it transforms with two factors of the inverse transpose of $ \mathbf{T} $$

* . Thus, it is a second-rank contravariant tensor: $ g^{ij} $$.

Notice how the position of the indices (subscript or superscript) immediately tells us the covariant or contravariant nature of the quantity. We no longer need to use separate symbols like $ g^{reciprocal}\_{ij}

$$ or $ \text{rg}\_{ij} $$

to distinguish the reciprocal space metric tensor; $ g^{ij} $$ clearly indicates its contravariant nature and its domain.

### 1.7.3. Example: Length of a Vector in Einstein Notation

Let’s revisit the square of the length (norm) of a vector $ = x^i \_i

$$.
We found it to be $ |\mathbf{r}|^2 = x^i x^j g\_{ij} $$

.

In Einstein notation, this becomes:

Here, $ i

$$ and $ j $$

are summation indices. The contravariant components $ x^i

$$ and $ x^j $$

are contracted with the covariant metric tensor $ g\_{ij} $$. The resulting quantity has no free indices, meaning it is a scalar. This immediately tells us that the square of the length of a vector is an **invariant scalar** quantity, independent of the chosen coordinate system. This is physically intuitive; the actual length of an object does not change just because we describe it using a different set of axes.

This clear visual representation of covariance, contravariance, and summation is a hallmark of tensor calculus and streamlines complex mathematical expressions in physics and materials science.

## 1.8. Covariance of Physical Equations

One of the profound implications of using covariant and contravariant tensor notation is the ability to immediately ascertain whether a physical equation is **covariant** (in the broader sense of maintaining its form under coordinate transformations).

### 1.8.1. Definition of Covariant Equations

An equation is said to be **covariant** if its form remains unchanged under a specified class of coordinate transformations. In tensor notation, this means that the **index structure** (i.e., the number and position of upper and lower indices) must be identical on both sides of the equation. If the index structure matches, it implies that both sides transform in the same way, thus preserving the equation’s physical meaning regardless of the chosen coordinate system.

This concept is paramount in modern physics, where physical laws are expected to be independent of the observer’s frame of reference.

### 1.8.2. Symmetry Principles and Physical Laws

The requirement for physical laws to be covariant is deeply intertwined with **symmetry principles**. Most fundamental physical laws are derived or formulated to obey certain symmetries. For example:

* **Translational invariance:** Physical laws don’t change if you shift your entire experiment to a different location in space.
* **Rotational invariance:** Physical laws don’t change if you rotate your coordinate system.
* **Lorentz invariance:** The laws of physics are the same for all observers in uniform motion relative to one another (special relativity).
* **General Covariance:** The laws of physics should be the same for all observers, regardless of their state of motion or the geometry of spacetime (general relativity).

When physical laws are expressed in a tensor formalism using covariant and contravariant components, the covariance of the equation (in terms of index matching) provides a direct visual check that the underlying symmetry is respected. If the left-hand side and right-hand side of a tensor equation have different index structures, the equation is not covariant and is likely physically inconsistent.

### 1.8.3. Examples from Physics

* **Special Relativity:** Maxwell’s equations and the laws of mechanics are formulated to be **Lorentz covariant**. This means they retain their form under Lorentz transformations, which relate different inertial frames of reference. The four-vector notation, which combines space and time into a single entity with covariant and contravariant components, naturally expresses this covariance.
* **General Relativity:** Einstein’s theory of general relativity is based on the principle of **general covariance**. Its equations, such as the Einstein field equations, are explicitly formulated using tensors (e.g., the metric tensor, Ricci tensor, energy-momentum tensor) such that they are covariant under *arbitrary* coordinate transformations, including those in curved spacetime.
* **String Theory:** In more advanced theories like string theory, theoretical physicists strive to construct theories that are not only Lorentz covariant but also possess other symmetries, such as **supersymmetry** and **worldsheet conformal invariance**. The Lagrangian (a scalar quantity from which equations of motion are derived) for such theories is carefully designed to exhibit these covariant and invariant properties.

By organizing physical equations using covariant and contravariant concepts, we gain tremendous clarity and predictive power. It allows physicists and materials scientists to design and analyze theoretical models with a built-in consistency check against fundamental symmetry principles.

## 1.9. Identifying Unknown Tensor Components

The power of tensor notation extends to situations where the covariant or contravariant nature of a quantity is initially unknown. By adhering to the index rules of a covariant equation, we can deduce the character of such unknown vectors or tensors.

Let’s consider the transformation of real-space basis vectors $ \_j

$$ to a new set $ \mathbf{a}'\_i $$

. We’ve previously written this as:

In standard Einstein notation, $ \_i

$$ and $ \mathbf{a}\_j $$

are covariant vectors (lower indices). For the equation to be covariant, the index structure must match. This means that on the right-hand side, the index $ j

$$ must be contracted. Therefore, the transformation matrix $ T\_{ij} $$

must have its $ j

$$ index as contravariant and its $ i $$

index as covariant.

So, the correct tensor notation for the transformation of basis vectors is:

Here, $ \_j

$$ is covariant. The index $ j $$

is summed over (one upper from $ T^j\_i

$$, one lower from $ \mathbf{a}\_j $$

). The remaining index $ i

$$ is lower on both sides. This signifies that $ T^j\_i $$

is a **mixed tensor of rank 2**, with one contravariant index $ j

$$ and one covariant index $ i $$

. This specific type of mixed tensor is responsible for transforming covariant vectors.

Similarly, for the transformation of reciprocal lattice basis vectors, which are contravariant ($ ^j

’^i = (T{-1})i\_j ^j

$$
Here, $ \mathbf{a}^j $$

is contravariant. The index $ j

$$ is summed over. The remaining index $ i $$

is upper on both sides. This signifies that $ (T{-1})i\_j

$$ is also a mixed tensor of rank 2, but with its contravariant index $ i $$

as a superscript and covariant index $ j $$ as a subscript. This tensor transforms contravariant vectors.

The crucial takeaway is that while we might use the symbol T\_ij in simple matrix algebra, in rigorous tensor calculus, the precise placement of indices ($ T^i\_j

$$, $ T\_{ij} $$

, or $ T^{ij}

$$) determines its transformation properties. This is similar to how $ g\_{ij} $$

and $ g^{ij} $$ both use g but their index positions clearly denote their covariant or contravariant nature.

### 1.9.1. Examples of Physical Tensors in Materials Science

Let’s apply this indexing strategy to other important tensors in materials science:

1. \*\*Dielectric Permittivity Tensor ($ *{ij} $$):\*\*
   The electric displacement field $ \mathbf{D} $$ and the electric field $ $$ are related by the dielectric permittivity tensor. A common way to express their relationship is via the electric energy density $ U $$, which is a scalar invariant: If we relate $ D^i $$ to $ E\_j $$, then $ D^i = ^{ij} E\_j $$, making $ \epsilon^{ij} $$ a contravariant tensor. Alternatively, if we consider $ D\_i =* {ij} E^j

$$, then $ \epsilon\_{ij} $$

* is a covariant tensor. The choice depends on the convention for $

$$ and $ \mathbf{E} $$

* . However, for the scalar energy density $ U = \_{ij} E^i E^j

$$, with $ E^i $$

* and $ E^j

$$ as contravariant components of the electric field vector, the dielectric permittivity tensor $ \epsilon\_{ij} $$

* must be a **second-rank covariant tensor** to yield a scalar quantity.

1. **Strain Tensor ($ *{ij} $$):\*\*
   The strain tensor describes the deformation of a material. It can be defined from the displacement gradient. If $ x^i $$ are contravariant coordinates and $ X^j $$ are the original coordinates, and $ u^i = x^i - X^i $$ is the displacement (a contravariant vector), then the displacement gradient $ u^i / X^j* {ij} = ( + ) $$
   Here, $ u\_i = g\_{ik} u^k $$ are covariant components of displacement, and $ / X^j $$ leads to a covariant index. Thus, the strain tensor $ \epsilon\_{ij} $$ is typically defined as a** second-rank covariant tensor\*\*.
2. **Elastic Constant Tensor (Stiffness Tensor, $ C\_{ijkl} $$):\*\*
   This tensor relates stress $ \sigma\_{ij} $$ to strain $ *{kl}* {ij} = C\_{ijkl} *{kl} $$
   Here, stress $ \sigma\_{ij} $$ and strain $* {kl} $$ are typically second-rank covariant tensors. For the equation to be covariant, the elastic constant tensor $ C\_{ijkl} $$ must therefore be a** fourth-rank covariant tensor\*\*. It has four lower indices because it maps two covariant indices ($ \_{kl}

$$) to two covariant indices ($ \sigma\_{ij} $$

* ) on the left-hand side.

This systematic use of index placement provides a powerful framework for developing and analyzing physical theories, ensuring consistency across different coordinate systems.

## 1.10. Tensor Components in Cartesian vs. Crystallographic Coordinates

While tensor notation provides a powerful, coordinate-independent way to express physical laws, in practical materials science, we often need to deal with actual numerical values of tensor components. These values depend on the specific coordinate system chosen.

* **Single Crystals:** For single crystals, the orientation of the unit cell axes ($ \_1, \_2, \_3

$$) defines a natural crystallographic coordinate system. It is straightforward to define tensor components with respect to these axes. For example, $ C\_{11} $$

* in an elastic stiffness matrix would refer to a stiffness component along the $ \_1

$$ direction (if $ \mathbf{a}\_1 $$

* were aligned with a principal axis).
* **Polycrystals:** For polycrystalline materials, where individual grains are randomly oriented, we often deal with averaged properties. To calculate these averages, the tensor components from individual grains (expressed in their crystallographic axes) must be transformed into a common reference frame (often a Cartesian laboratory frame), averaged, and then potentially back-transformed or diagonalized to find principal values. This process involves complex tensor rotations.

### 1.10.1. Computational Material Science and Cartesian Coordinates

In computational materials science, particularly with *ab initio* simulation packages like **VASP (Vienna Ab initio Simulation Package)**, a common practice is to output tensor components (e.g., elastic constants, dielectric tensors, Born effective charges) not directly with respect to the crystallographic primitive vectors but with respect to a **fixed Cartesian coordinate system**.

**Why Cartesian Coordinates?** \* **Simplicity:** Cartesian coordinates (X, Y, Z axes, all mutually orthogonal and of unit length) simplify tensor algebra significantly. The metric tensor in a Cartesian system is simply the identity matrix ($ \_{ij}

$$), meaning there's no distinction between covariant and contravariant components ($ g\_{ij} = g^{ij} = \delta\_{ij} $$

). \* **Interoperability:** It provides a universal reference frame for comparing calculations from different systems or with experimental data, regardless of the crystal’s specific lattice parameters or angles.

**How VASP defines Cartesian coordinates:** VASP, for example, typically defines its Cartesian coordinate system based on the input lattice vectors provided in the POSCAR file. \* The first lattice vector (e.g., A1 in POSCAR) is usually aligned along the X-axis. \* The second lattice vector (A2) lies in the XY-plane. \* The third lattice vector (A3) completes the 3D basis (often by being perpendicular to the XY-plane if the crystal structure allows, or adjusted to form a right-handed system).

All subsequent property tensors calculated by VASP are then reported with respect to *this* internally defined Cartesian coordinate system. This means that to interpret VASP outputs in terms of crystallographic directions (e.g., [100] or [111] in cubic systems), one must perform an appropriate coordinate transformation (rotation) from the Cartesian frame back to the desired crystallographic frame.

This practice underscores the importance of understanding coordinate transformations and tensor properties, even when working with seemingly “simple” Cartesian outputs from computational tools.

## 1.11. Summary of Covariant and Contravariant Rules

Let’s consolidate the fundamental rules governing covariant and contravariant quantities. Mastering these rules is key to correctly applying tensor calculus in materials science.

### 1.11.1. Core Rules for Covariance and Contravariance

1. **Basis Vectors vs. Coordinates:**
   * If basis vectors are **covariant** (e.g., real-space primitive vectors $ \_i

$$), their corresponding components (coordinates) are \*\*contravariant\*\* (e.g., $ x^i $$

* + ). A vector $

$$ is then $ \mathbf{R} = x^i \mathbf{a}\_i $$

* + .
  + Conversely, if basis vectors are **contravariant** (e.g., reciprocal-space primitive vectors $ ^i

$$), their corresponding components (coordinates) are \*\*covariant\*\* (e.g., $ h\_i $$

* + ). A vector $

$$ is then $ \mathbf{R} = h\_i \mathbf{a}^i $$

* + .

1. **Real Space vs. Reciprocal Space:**
   * The real-space primitive basis vectors $ \_i $$ are typically treated as **covariant**.
   * The reciprocal-space primitive basis vectors $ ^i

$$ are typically treated as \*\*contravariant\*\*.
This duality is a direct consequence of their definition ($ \mathbf{a}^i \cdot \mathbf{a}\_j = 2\pi \delta^i\_j $$

* + ).

1. **Differentiation:**
   * Taking the gradient with respect to a contravariant coordinate ($ /x^i

$$) results in a \*\*covariant\*\* quantity. Example: $ \frac{\partial \phi}{\partial x^i} $$

* + (the components of the gradient of a scalar field $ $$) are covariant.
  + Taking the gradient with respect to a covariant coordinate ($ /x\_i $$) results in a **contravariant** quantity. This means that a derivative “lowers” an index if taken with respect to an upper-indexed variable, and “raises” it if taken with respect to a lower-indexed variable.

1. **Role of the Metric Tensor (Index Lowering/Raising):**
   * The covariant metric tensor $ g\_{ij}
   * X\_i = g\_{ij} X^j $$
   * The contravariant metric tensor $ g^{ij}
   * X^i = g^{ij} X\_j $$ This is often referred to as “raising and lowering indices” and is fundamental for transforming components between their covariant and contravariant forms.

Here is a summary table:

| Quantity | Index Type | Example of Einstein Notation | Transformation Rule (conceptual) |
| --- | --- | --- | --- |
| Real-space basis vector | Covariant | $ \_i  $$ | Transforms like $ T^j\_i $$ |  |
| Real-space coordinate | Contravariant | $ x^i  $$ | Transforms like $ (T^{-1})^i\_j $$ |  |
| Reciprocal-space basis vector | Contravariant | $ ^i  $$ | Transforms like $ (T^{-1})^i\_j $$ |  |
| Reciprocal-space coordinate | Covariant | $ h\_i  $$ | Transforms like $ T^j\_i $$ |  |
| Covariant Metric Tensor | Covariant (rank 2) | $ g\_{ij}  $$ | Transforms like $ T^k\_i T^l\_j $$ |  |
| Contravariant Metric Tensor | Contravariant (rank 2) | $ g^{ij}  $$ | Transforms like $ (T^{-1})^i\_k (T^{-1})^j\_l $$ |  |
| Gradient of Scalar Field | Covariant | $ \_i = $$ | (Transforms as covariant vector) |

By consistently applying these rules and the Einstein summation convention, you can confidently perform calculations and derive relationships involving tensors, ensuring their validity across different coordinate systems. This rigorous approach is a hallmark of advanced materials science and condensed matter physics.

## 1.12. Geometric Interpretation of Covariant and Contravariant Coordinates

To conclude our discussion, let’s look at the geometric meaning of covariant and contravariant coordinates, which can sometimes be a source of confusion. The distinction lies in how a vector is projected onto or resolved by the basis vectors.

Consider a 2D vector $

$$ and a set of oblique (non-orthogonal) real-space basis vectors $ \mathbf{a}\_1 $$

and $ \_2 $$.

### 1.12.1. Contravariant Coordinates (Parallel Projection)

When we write $ = x^1 \_1 + x^2 \_2

$$, the components $ x^1 $$

and $ x^2

$$ are the \*\*contravariant coordinates\*\*. Geometrically, these are found by performing \*\*parallel projections\*\*:
1. Draw a line from the tip of $ \mathbf{r} $$

parallel to $ \_2

$$ until it intersects the line defined by $ \mathbf{a}\_1 $$

. The length along $ \_1

$$ from the origin to this intersection point, normalized by $ |\mathbf{a}\_1| $$

, gives $ x^1

$$.
2. Similarly, draw a line from the tip of $ \mathbf{r} $$

parallel to $ \_1

$$ until it intersects the line defined by $ \mathbf{a}\_2 $$

. The length along $ \_2

$$ from the origin to this intersection point, normalized by $ |\mathbf{a}\_2| $$

, gives $ x^2 $$.

This is essentially resolving the vector $ $$ into components *along* the basis vectors themselves. This is the standard way we often think about components in an oblique coordinate system.

### 1.12.2. Covariant Coordinates (Orthogonal Projection using Reciprocal Basis)

Now, let’s consider the reciprocal lattice basis vectors $ ^\*\_1

$$ and $ \mathbf{a}^\*\_2 $$

. Recall that $ ^\*\_1

$$ is perpendicular to $ \mathbf{a}\_2 $$

, and $ ^\*\_2

$$ is perpendicular to $ \mathbf{a}\_1 $$

.

If we consider the representation $ = x\_i ^i

$$, where $ \mathbf{a}^i $$

are the contravariant reciprocal basis vectors, then $ x\_i $$ are the covariant components.

Geometrically, the covariant component $ x\_1

$$ of vector $ \mathbf{r} $$

can be found by taking the dot product $ (^\*\_1 / 2)

$$. This means that the covariant components correspond to the \*\*orthogonal projection\*\* of $ \mathbf{r} $$

onto the directions of the *reciprocal* lattice vectors.

Specifically, for a vector $

$$, its covariant components $ x\_1, x\_2 $$

can be found by:

(The $ 2

$$ factor may be omitted depending on the convention for $ \mathbf{a}^\*\_i $$

).

This means that: \* **Contravariant components** ($ x^i

$$) represent the lengths along the skewed axes of the real lattice (parallel projection). They indicate "how much of each basis vector" is needed to construct the vector.
\* \*\*Covariant components\*\* ($ x\_i $$

) represent the lengths obtained by orthogonal projection onto the directions defined by the reciprocal lattice vectors. They indicate the “projection onto the plane normal to the other basis vectors.”

The metric tensor $ g\_{ij}

$$ (or $ g^{ij} $$

) acts as the bridge between these two types of coordinates, allowing us to convert between parallel projections and orthogonal projections, effectively shifting between viewing a vector in terms of real-space basis vectors or reciprocal-space basis vectors.

Understanding this geometric distinction is crucial for fully appreciating the power and utility of covariant and contravariant tensor notation in describing the properties of crystalline materials.