材料科学数学基础

2013年9月

北京大学深圳研究生院

课程介绍

- **2013秋季学期**
- **任课教师：陶国华**

  网页 http://web.pkusz.edu.cn/taoguohua
- 材料专业必修课　48学时3学分
- **教材：**讲义
- **参考书：**Mathematical Methods for Physicists, George B. Arfken and Hans J. Weber, Academic Press.
  - 网络资源：如Wikipedia
- **答疑时间：**周三下午4-5点 G栋308
- **评分标准：**口试（50%）、期末考试（50%）
- **口试形式：**每人20分钟（报告15分钟+提问5分钟），题目可从备选题目中选取，亦可自行选取（需征得任课教师同意后方可实施）。**口试讲稿必须于第十周提交**。

理想

为天地立心

为生民立命

为往圣继绝学

为万世开太平

为何而读书？

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科技与材料

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定性与定量

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火药

Chapter 1: Vector Analysis

Scalar and vector

- Scalar

  number

- Vector

  a number + its “direction”

  ex. $\vec{F} = m\vec{a}$

A vector **v** may be represented by many different ways
Ex. (see right)
$\mathbf{v} = x\mathbf{e}_1 + y\mathbf{e}_2$
or $\mathbf{v} = \mathbf{f}_1 + \mathbf{f}_2$

The **basis** (linear independent vectors) defines the direction.

Properties

- Addition

    triangle law

- Commutative

    parallelogram law

    C=A+B=B+A

- Associative

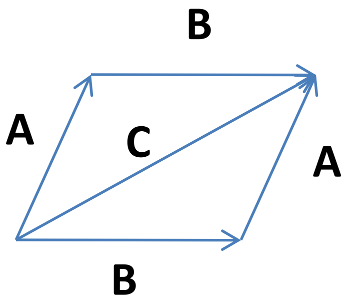
    D=A+B+C

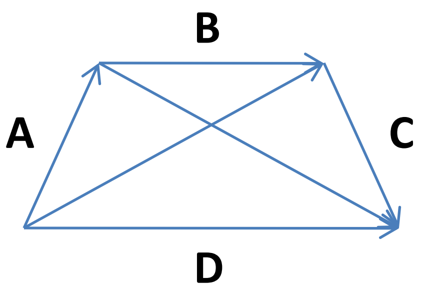
    =(A+B)+C=A+(B+C)

- Distributive

    $a(\mathbf{u} + \mathbf{v}) = a\mathbf{u} + a\mathbf{v}$

    $(a + b)\mathbf{v} = a\mathbf{v} + b\mathbf{v}$





Coordinate

- Direction cosine

$A_{x,y,z}$ components (projections) of A

- Scalar product

$$\vec{A}\cdot\vec{B} = |A||B|\cos\theta_{AB}$$

$$|A|^2 = A_x^2 + A_y^2 + A_z^2$$

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- Unit vector

$$\hat{i} = \frac{\hat{x}}{|x|}$$

- Orthogonality

$$\vec{A}\cdot\vec{B} = 0$$

Standard basis (orthonormal)
Normal vector (of a plane)

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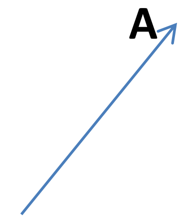
Vector space

The collection of vectors forms vector space. And it has the following properties:

1. Vector equality
   1. **A**=**B =>** $A_i=B_i$
2. Addition
   1. Associativity (**A**+**B**)+**C**=**A**+(**B+C**)
   2. Commutativity **A+B=B+A**
   3. Distributivity a*(**A+B**)=a*__A__+a*__B__; (a+b)*__A__=a*__A__+a*__B__
3. Scalar multiplication
   1. Compatibility a*(b*__A__)=(a*b)*__A__
   2. Identity element 1*__A__=**A**
4. Negative of a vector (inverse element)
   A+(-**A**)=0
5. Null vector (identity element of addition)
   A+0=**A** for any **A**

Rotation

Take the 2D space for simplicity, for any vector **A**, its new representation in a rotated axes is given by



$$\begin{bmatrix} A'_x \\ A'_y \end{bmatrix} = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \begin{bmatrix} A_x \\ A_y \end{bmatrix}$$

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Rotate the vector instead of the coordinate

$$\begin{bmatrix} A_x \\ A_y \end{bmatrix} = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}^{-1} \begin{bmatrix} A'_x \\ A'_y \end{bmatrix}$$

$$= \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{bmatrix} A'_x \\ A'_y \end{bmatrix}$$

Orthogonal matrix

$$U = \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}$$

$$UU^{-1} = I$$

Orthogonal condition: $\sum_i a_{ij} a_{ik} = \delta_{ik}$

Rotation

- Scalar is rotational invariant.
  - 1
    $$A^2 = A'^2 = \sum_i A_i^2 = \sum_i A_i'^2$$
    $$= \sum_i \left(\sum_j a_{ij} A_j \right) \left(\sum_k a_{ik} A_k \right) = \sum_{j,k} A_j A_k \sum_i a_{ij} a_{ik}$$
    $$\Leftrightarrow \sum_i a_{ij} a_{ik} = \delta_{ik}$$
  - 2
    $$A' \cdot B' = \sum_i A_i' B_i'$$
    $$= \sum_i \left(\sum_j a_{ij} A_j \right) \left(\sum_k a_{ik} B_k \right) = \sum_{j,k} A_j B_k \sum_i a_{ij} a_{ik}$$
    $$= \sum_j A_j B_j = A \cdot B$$
  - 2'
    $$C = A + B$$
    $$C \cdot C = (A+B) \cdot (A+B) = A \cdot A + B \cdot B + 2A \cdot B$$

3D Rotation

- Rotational matrix

$$U = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}$$

3D rotation described by three steps defined by Euler angles

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$$A(\alpha,\beta,\gamma) = R_z(\gamma)R_y(\beta)R_z(\alpha)$$

$$= \begin{pmatrix} \cos\gamma & \sin\gamma & 0 \\ -\sin\gamma & \cos\gamma & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \cos\beta & 0 & -\sin\beta \\ 0 & 1 & 0 \\ \sin\beta & 0 & \cos\beta \end{pmatrix} \begin{pmatrix} \cos\alpha & \sin\alpha & 0 \\ -\sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$= \begin{pmatrix} \cos\gamma\cos\beta\cos\alpha - \sin\gamma\cos\alpha & \cos\gamma\cos\beta\sin\alpha + \sin\gamma\cos\alpha & -\cos\gamma\sin\beta \\ -\sin\gamma\cos\beta\cos\alpha - \cos\gamma\sin\alpha & -\sin\gamma\cos\beta\sin\alpha + \cos\gamma\cos\alpha & \sin\gamma\sin\beta \\ \sin\beta\cos\alpha & \sin\beta\sin\alpha & \cos\beta \end{pmatrix}$$

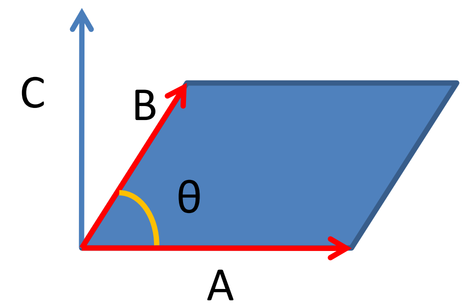
Vector product

Geometric definition:

$$C = A \times B$$
$$|C| = |A||B|\sin\theta$$

Algebraic definition:

$$C = A \times B$$
$$= \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ A_x & A_y & A_z \\ B_x & B_y & B_z \end{vmatrix}$$



Area of parallelogram

The equivalence of the two:

$$C^2 = (A \times B)\cdot(A \times B) = A^2B^2 - (A \cdot B)^2$$
$$= A^2B^2 - A^2B^2\cos^2\theta = A^2B^2\sin^2\theta$$

Ex.

Anticommutation: $A \times B = -B \times A$

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Triple product:

$$C \cdot (A \times B)$$
$$= \begin{vmatrix} C_x & C_y & C_z \\ A_x & A_y & A_z \\ B_x & B_y & B_z \end{vmatrix}$$

$$A \times (B \times C) = (A \cdot C)B - (A \cdot B)C$$

The volume of the parallelepiped

Reciprocal lattice

The inverse of the Bravais lattice consists of the set of wave vectors ***K***

$$e^{iK\cdot R}=1$$ for all real space vectors ***R***

$$b_1 = 2\pi \frac{a_2 \times a_3}{a_1 \cdot (a_2 \times a_3)}$$

$$b_2 = 2\pi \frac{a_3 \times a_1}{a_2 \cdot (a_3 \times a_1)}$$

$$b_3 = 2\pi \frac{a_1 \times a_2}{a_3 \cdot (a_1 \times a_2)}$$

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