

Quantum Mechanics_polarization density

In classical electromagnetism, **polarization density** (or **electric polarization**, or simply **polarization**) is the vector field that expresses the density of permanent or induced electric dipole moments in a dielectric material. When a dielectric is placed in an external Electric field, its molecules gain Electric dipole moment and the dielectric is said to be polarized. The electric dipole moment induced per unit volume of the dielectric material is called the electric polarization of the dielectric.[1][2]

Polarization density also describes how a material responds to an applied electric field as well as the way the material changes the electric field, and can be used to calculate the forces that result from those interactions. It can be compared to Magnetization, which is the measure of the corresponding response of a material to a Magnetic field in Magnetism. The SI unit of measure is coulombs per square metre, and polarization density is represented by a vector **P**. [3]

Definition

The polarization density **P** is defined as the average Electric dipole moment **d** per unit volume *V* of the dielectric material: [4]

$$\mathbf{P} = \frac{\langle \mathbf{d} \rangle}{V}$$

which can be interpreted as a measure of how strong and how aligned the dipoles are in a region of the material. For the calculation of **P** due to an applied electric field, the electric susceptibility χ of the dielectric must be known (see below).

Polarization density in Maxwell's equations

The behavior of electric fields (**E** and **D**), magnetic fields (**B**, **H**), charge density (ρ) and current density (**J**) are described by Maxwell's equations in matter. The role of the polarization density **P** is described below.

Relations between E, D and P

The polarization density **P** yields the electric displacement field **D** via [5]

$$\mathbf{D} = \epsilon_0 \mathbf{E} + \mathbf{P}.$$

Here ϵ_0 is the electric permittivity of empty space. In this equation, **P** is the (negative of the) field induced in the material when the "fixed" charges, the dipoles, shift in

response to the total underlying field \mathbf{E} , whereas \mathbf{D} is the field due to the remaining charges, known as "free" charges. In general, \mathbf{P} varies as a function of \mathbf{E} depending on the medium, as described later in the article. In many problems, it is more convenient to work with \mathbf{D} and the free charges than with \mathbf{E} and the total charge.[6]

Bound charge

Electric polarization corresponds to a realignment of the bound electrons in the material (i.e., bound to a molecule), which creates an additional charge density, known as the **bound charge density** ρ_b : [7]

$$\rho_b = -\nabla \cdot \mathbf{P}$$

so that the total charge density that enters Maxwell's equation for the divergence of \mathbf{E} is given by

$$\rho = \rho_f + \rho_b$$

where ρ_f is the **free charge density** given by the divergence of \mathbf{D} .

At the surface of the polarized material, the bound charge appears as a surface charge density with $\hat{\mathbf{n}}_{\text{out}}$ as the normal vector: [8]

$$\sigma_b = \mathbf{P} \cdot \hat{\mathbf{n}}_{\text{out}}$$

If \mathbf{P} is uniform inside the material, this surface charge is the only bound charge. This can be seen from the above relation between \mathbf{P} and ρ_b ; if \mathbf{P} is uniform throughout the interior of some volume, its divergence in that volume must vanish.

When the polarization density changes with time, the time-dependent bound-charge density creates a polarization current density of

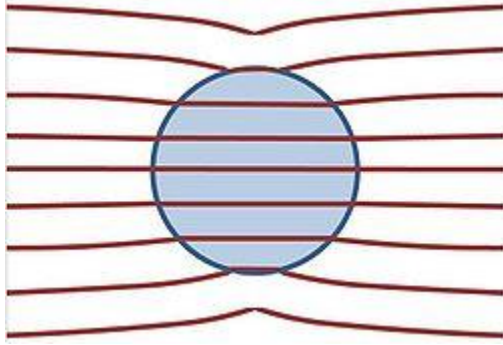
$$\mathbf{J}_p = \frac{\partial \mathbf{P}}{\partial t}$$

so that the total current density that enters Maxwell's equations is given by

$$\mathbf{J} = \mathbf{J}_f + \nabla \times \mathbf{M} + \frac{\partial \mathbf{P}}{\partial t}$$

where \mathbf{J}_f is the free-charge current density, and the second term is the magnetization current density (also called the *bound current density*), a contribution from atomic-scale magnetic dipoles (when they are present).

Relation between \mathbf{P} and \mathbf{E} in various materials



Field lines of the D-field in a dielectric sphere with greater susceptibility than its surroundings, placed in a previously-uniform field.[9] The Field lines of the E-field are not shown: These point in the same directions, but many field lines start and end on the surface of the sphere, where there is bound charge. As a result, the density of E-field lines is lower inside the sphere than outside, which corresponds to the fact that the E-field is weaker inside the sphere than outside.

In a homogeneous linear and isotropic dielectric medium, the **polarization** is aligned with and proportional to the electric field E:[10]

$$\mathbf{P} = \epsilon_0 \chi \mathbf{E},$$

where ϵ_0 is the electric constant, and χ is the electric susceptibility of the medium. Note that χ is just a scalar. This is a particular case due to the *isotropy* of the dielectric. This simply means that in this class of materials the polarization density is always parallel to the applied electric field. In general, χ is seen as a matrix that is applied to E. This class of dielectrics where the polarization density and the electric field are not in the same direction is known as anisotropic materials.

In such materials, the i^{th} component of the polarization is related to the j^{th} component of the electric field according to:[11]

$$P_i = \sum_j \epsilon_0 \chi_{ij} E_j,$$

This relation shows, for example, that a material can polarize in the x direction by applying a field in the z direction, and so on. The case of an anisotropic dielectric medium is described by the field of crystal optics.

As in most electromagnetism, this relation deals with macroscopic averages of the fields and dipole density, so that one has a continuum approximation of the dielectric materials that neglects atomic-scale behaviors. The polarizability of individual particles in the medium can be related to the average susceptibility and polarization density by the Clausius-Mossotti relation.

In general, the susceptibility is a function of the frequency ω of the applied field. When the field is an arbitrary function of time t , the polarization is a convolution of the Fourier transform of $\chi(\omega)$ with the $E(t)$. This reflects the fact that the dipoles in the material cannot respond instantaneously to the applied field, and causality considerations lead to the Kramers-Kronig relations.

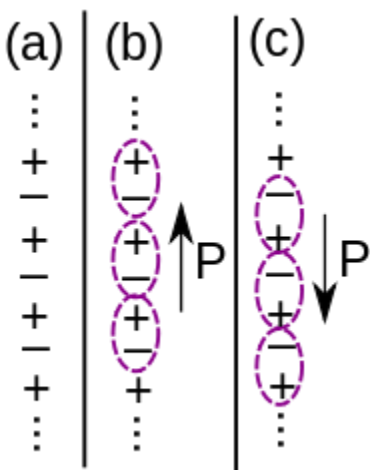
If the polarization \mathbf{P} is not linearly proportional to the electric field \mathbf{E} , the medium is termed *nonlinear* and is described by the field of nonlinear optics. To a good approximation (for sufficiently weak fields, assuming no permanent dipole moments are present), \mathbf{P} is usually given by a Taylor series in \mathbf{E} whose coefficients are the nonlinear susceptibilities:

$$\frac{P_i}{\epsilon_0} = \sum_j \chi_{ij}^{(1)} E_j + \sum_{jk} \chi_{ijk}^{(2)} E_j E_k + \sum_{jkl} \chi_{ijkl}^{(3)} E_j E_k E_l + \dots$$

where $\chi^{(1)}$ is the linear susceptibility, $\chi^{(2)}$ is the second-order susceptibility (describing phenomena such as the Pockels effect, optical rectification and second-harmonic generation), and $\chi^{(3)}$ is the third-order susceptibility (describing third-order effects such as the Kerr effect and electric field-induced optical rectification).

In ferroelectric materials, there is no one-to-one correspondence between \mathbf{P} and \mathbf{E} at all because of hysteresis.

Polarization ambiguity



Example of how the polarization density in a bulk crystal is ambiguous. (a) A solid crystal. (b) By pairing the positive and negative charges in a certain way, the crystal appears to have an upward polarization. (c) By pairing the charges differently, the crystal appears to have a downward polarization.

The polarization inside a solid is not, in general, uniquely defined: It depends on which electrons are paired up with which nuclei.[12] (See figure.) In other words, two people, Alice and Bob, looking at the same solid, may calculate different values of \mathbf{P} , and neither of them will be wrong. Alice and Bob will agree on the microscopic electric field \mathbf{E} in the solid, but disagree on the value of the displacement field $\mathbf{D} = \epsilon_0 \mathbf{E} + \mathbf{P}$. They will both find that Gauss's law is correct ($\nabla \cdot \mathbf{D} = \rho_{\text{free}}$), but they will disagree on the value of ρ_{free} at the surfaces of the crystal. For example, if Alice interprets the bulk solid to consist of dipoles with positive ions above and negative ions below, but the real crystal has negative ions as the topmost surface, then Alice will say that there is a negative free charge at the topmost surface. (She might view this as a type of surface reconstruction).

On the other hand, even though the value of \mathbf{P} is not uniquely defined in a bulk solid, *variations* in \mathbf{P} are uniquely defined.[12] If the crystal is gradually changed from one structure to another, there will be a current inside each unit cell, due to the motion of nuclei and electrons. This current results in a macroscopic transfer of charge from one side of the crystal to the other, and therefore it can be measured with an ammeter (like any other current) when wires are attached to the opposite sides of the crystal. The time-integral of the current is proportional to the change in \mathbf{P} . The current can be calculated in computer simulations (such as density functional theory); the formula for the integrated current turns out to be a type of Berry's phase. [12]

The non-uniqueness of \mathbf{P} is not problematic, because every measurable consequence of \mathbf{P} is in fact a consequence of a continuous change in \mathbf{P} . [12] For example, when a material is put in an electric field \mathbf{E} , which ramps up from zero to a finite value, the material's electronic and ionic positions slightly shift. This changes \mathbf{P} , and the result is electric susceptibility (and hence permittivity). As another example, when some crystals are heated, their electronic and ionic positions slightly shift, changing \mathbf{P} . The result is pyroelectricity. In all cases, the properties of interest are associated with a *change* in \mathbf{P} .

Even though the polarization is *in principle* non-unique, in practice it is often (not always) defined by convention in a specific, unique way. For example, in a perfectly centrosymmetric crystal, \mathbf{P} is usually defined by convention to be exactly zero. As another example, in a ferroelectric crystal, there is typically a acentrosymmetric configuration above the Curie temperature, and \mathbf{P} is defined there by

convention to be zero. As the crystal is cooled below the Curie temperature, it shifts gradually into a more and more non-centrosymmetric configuration. Since gradual changes in \mathbf{P} are uniquely defined, this convention gives a unique value of \mathbf{P} for the ferroelectric crystal, even below its Curie temperature.

References and notes

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