Response Functions

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- Electromagnetic spectrum;
- waves, photons, energy and momentum, flux;
- polarization of matter, optical functions and their relationships;
- example: polar (/doped) semiconducting crystal – GaAs.

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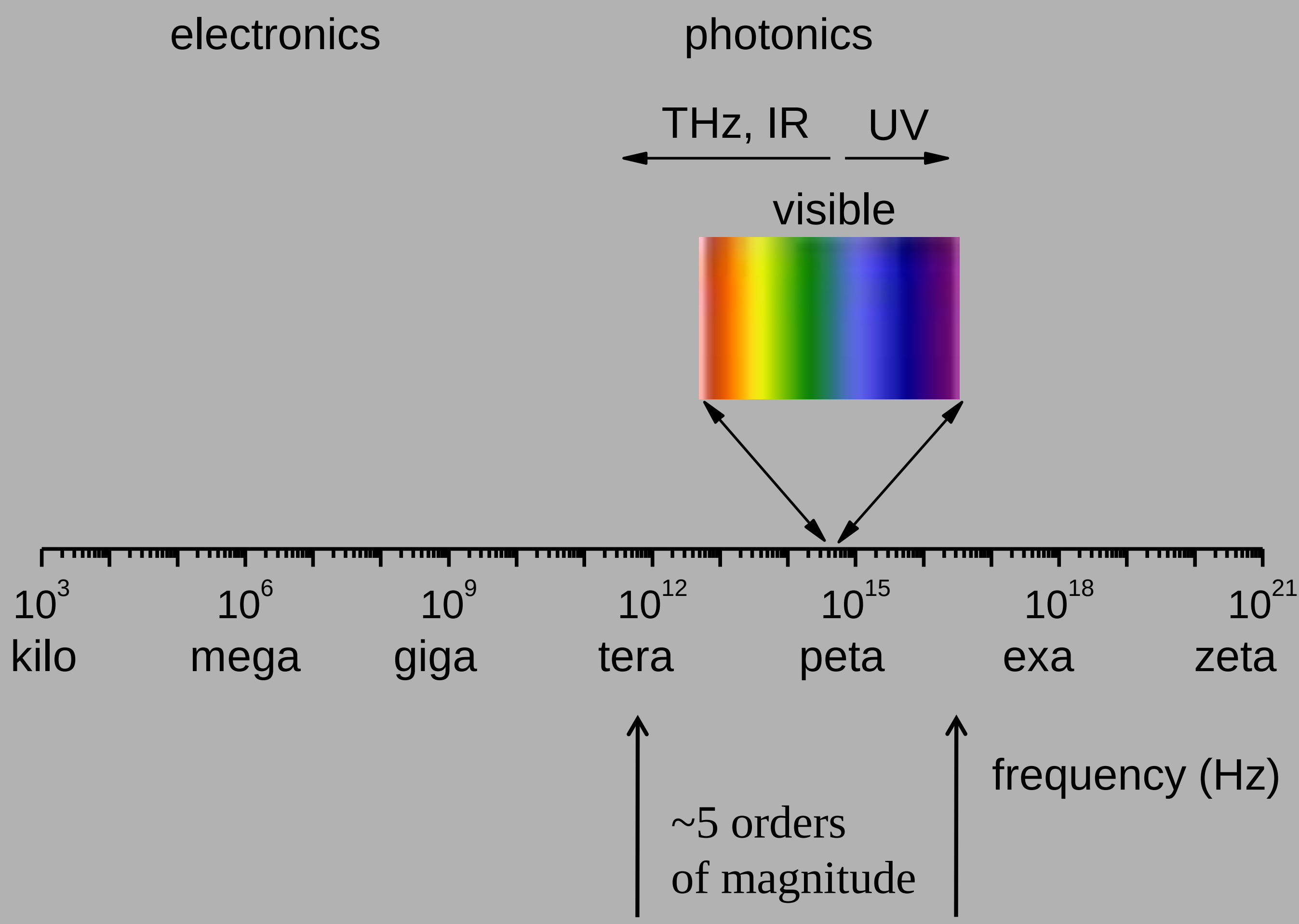
Optical frequencies of the electromagnetic spectrum

$$1\,\text{PHz} \propto 1\,\text{fs} \propto 0.3\,\mu\text{m} \propto 33000\,\text{cm}^{-1} \propto 4.1\,\text{eV} \propto 48000\,\text{K}$$



Electromagnetic waves

Harmonic oscillations at a fixed point in space,

$$\overrightarrow{E}(t) = \overrightarrow{E_0} e^{-i2\pi ft} = \overrightarrow{E_0} e^{-i\omega t},$$

wavy pattern in space-time, like the simple plane wave, propagating along the unit vector k_0:

$$\overrightarrow{E}(\vec{r},t) = \overrightarrow{E}_0 e^{-i(\omega t - 2\pi \vec{k}_0 \vec{r}/\lambda)} = \overrightarrow{E}_0 e^{-i(\omega t - \vec{k}\vec{r})}.$$

The basic charateristics:

electric intensity E (V/m),

frequency $f = \omega/2\pi$ (Hz),

wavelength $\lambda = c/f$ (μm, nm),

wavenumber $W = 1/\lambda$ (cm^{-1}).

Quantum behavior (Planck + Einstein):

photon energy $\hbar\omega$ (eV, K - from the corresponding temperature T, $= k_B T$),

momentum $\hbar\omega/c$ (eVs/m).

Electromagnetic waves

Wavelength - photon energy - wavenumber conversions:

$$\hbar\omega\ (\mathrm{eV}) = \frac{1.239852}{\lambda\ (\mu\mathrm{m})},\quad W\ (\mathrm{cm}^{-1}) = 8065.48\hbar\omega\ (\mathrm{eV}).$$

The light-matter interaction is governed by the electric field *E* of the wave; however, the signals measured by detectors are proportional to intensity, the time-averaged Poynting vector:

$$I = |\langle \vec{E}(t)\times\vec{H}(t)\rangle| = \frac{c\varepsilon_0}{2}|\vec{E}_0|^2.$$

Using the value $c\varepsilon_0$ = 0.002654 A/V, we find the following relations:
a wave with the electric field amplitude of 1V/m has the intensity of 1.33 mW/m^2;
a wave with the intensity of 1 mW/μm^2 has the amplitude of the electric intensity of 8.68×10^5 V/m.
This can be compared with the magnitude of the intensity of the field of one elementary charge at the distance of 0.1 nm, which is 1.44×10^{11} V/m.

Electromagnetic waves - quantum behavior

The classical picture of the electromagnetic wave fails on many occasions.

The flow of energy has to be treated as a train of quanta (photons); the intensity I and power P of a monochromatic beam are

$$I = \hbar\omega \times \text{(number of photons per units of area and time),}$$

$$P = \hbar\omega \times \text{(number of photons per unit of time).}$$

For example, the red HeNe laser line of λ=632.8 nm is composed of the 1.959 eV quanta. The power of 1 mW corresponds to the flux of 3.19×10^{18} photons per second.

State-of-the art detectors operate at the dark noise level of about 10 elementary charges (that can be produced by a slightly higher number of photons) → it is fairly easy to observe the linear response of matter (the number of absorbed photons proportional to the number of incoming photons).

Polarization of matter

The electric field of the light wave moves the atomic nuclei and electrons in our samples;

the movements are typically asynchronous, with “phase shifts” between the external force (proportional to the electric intensity *E*) and the induced oscillating dipole moments (or, equivalently, induced currents), with pronounced dependence on the (angular) frequency ω;

complex numbers keep track of the amplitudes and phases

(ellipsometry provides two real numbers at each frequency);

in weak fields, the response is linear (*D* is induction, *P* is polarization, χ is susceptibility, ε is permittivity, *j* is induced current, *σ* is conductivity):

$$\vec{D} \equiv \varepsilon_0 \vec{E} + \vec{P} = (1 + \hat{\chi})\varepsilon_0 \vec{E} = \hat{\varepsilon}\varepsilon_0 \vec{E}$$

$$\vec{j} = -i\omega \vec{P} = \sigma \vec{E}$$

Relationships between optical constants

Optical Constant (symbol)	Real part	Imaginary part
conductivity ($\sigma = \sigma_1 + i\sigma_2$)	$\sigma_1 = \omega\varepsilon_0\varepsilon_2$	$\sigma_2 = -\omega\varepsilon_0(\varepsilon_1 - 1)$
dielectric function ($\varepsilon = \varepsilon_1 + i\varepsilon_2$)	$\varepsilon_1 = 1 - \sigma_2/(\omega\varepsilon_0)$ $\varepsilon_1 = n^2 - k^2$	$\varepsilon_2 = \sigma_1/(\omega\varepsilon_0)$ $\varepsilon_2 = 2nk$
refractive index ($N = n + ik$)	$n = \sqrt{(\varepsilon_1 + \sqrt{\varepsilon_1^2 + \varepsilon_2^2})/2}$ $n = \varepsilon_2/(2k)$	$k = \sqrt{(-\varepsilon_1 + \sqrt{\varepsilon_1^2 + \varepsilon_2^2})/2}$ $k = \varepsilon_2/(2n)$
negative inverse of dielectric function ($-\varepsilon^{-1}$)	$-\varepsilon_1/(\varepsilon_1^2 + \varepsilon_2^2)$	$\varepsilon_2/(\varepsilon_1^2 + \varepsilon_2^2)$

The real part of conductivity (imaginary part of dielectric function) is a measure of absorbed energy;

the imaginary part of the refractive index is a measure of the attenuation of the light wave.

SI units

D	(F/m)·(V/m)=C/m^2
P	C/m^2
j	A/m^2
ED	(V/m)·(A·s/m^2)=J/m^3
I	(V/m)·(A/m)= W/m^2
χ, ε	dimensionless
σ	(A/m^2)/(V/m)=1/(Ωm)

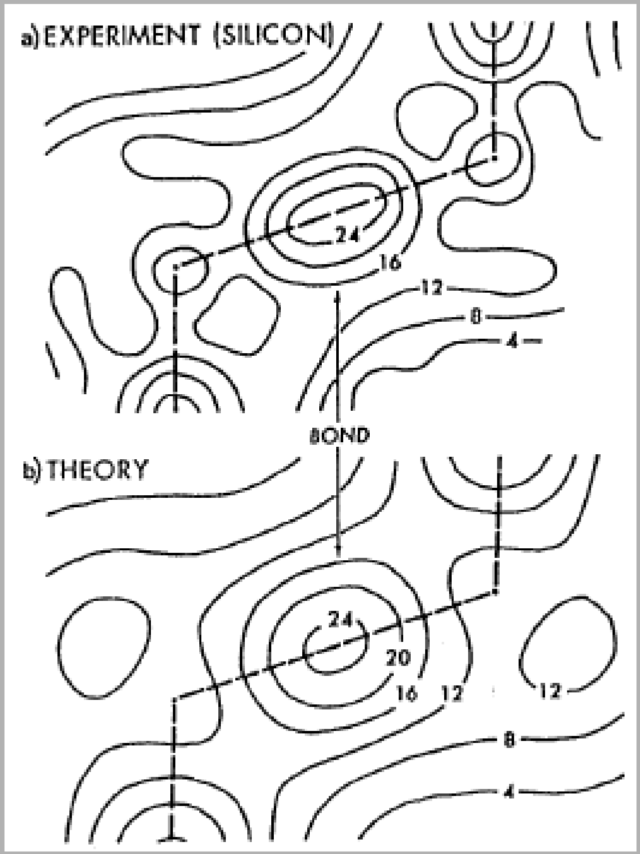
Example: polar (/doped) semiconducting crystal - GaAs

Electron density in the ground state

(Cohen and Chellikowsky, Electronic Structure and Optical Properties of Semiconductors, nonlocal pseudopotential)

suggests a difference in the IR response due to lattice vibrations

Si



GaAs

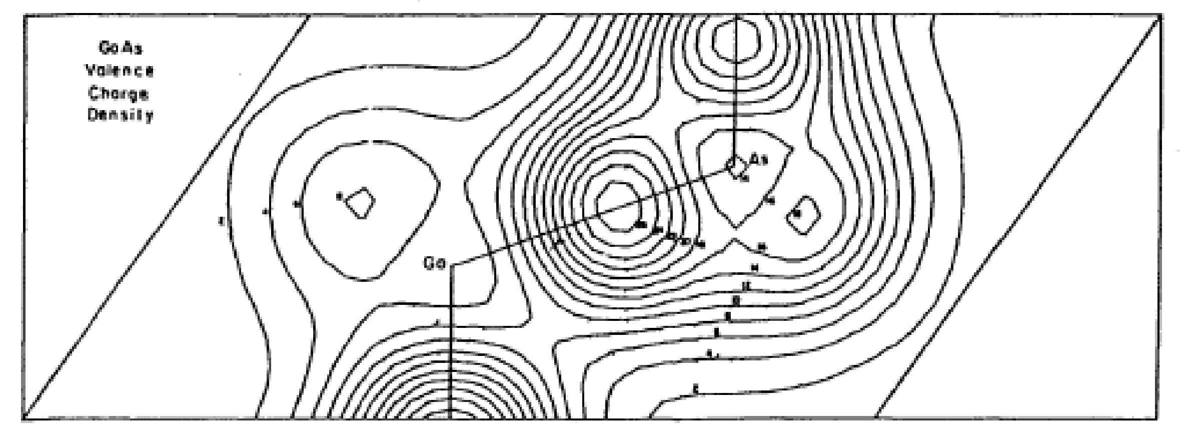
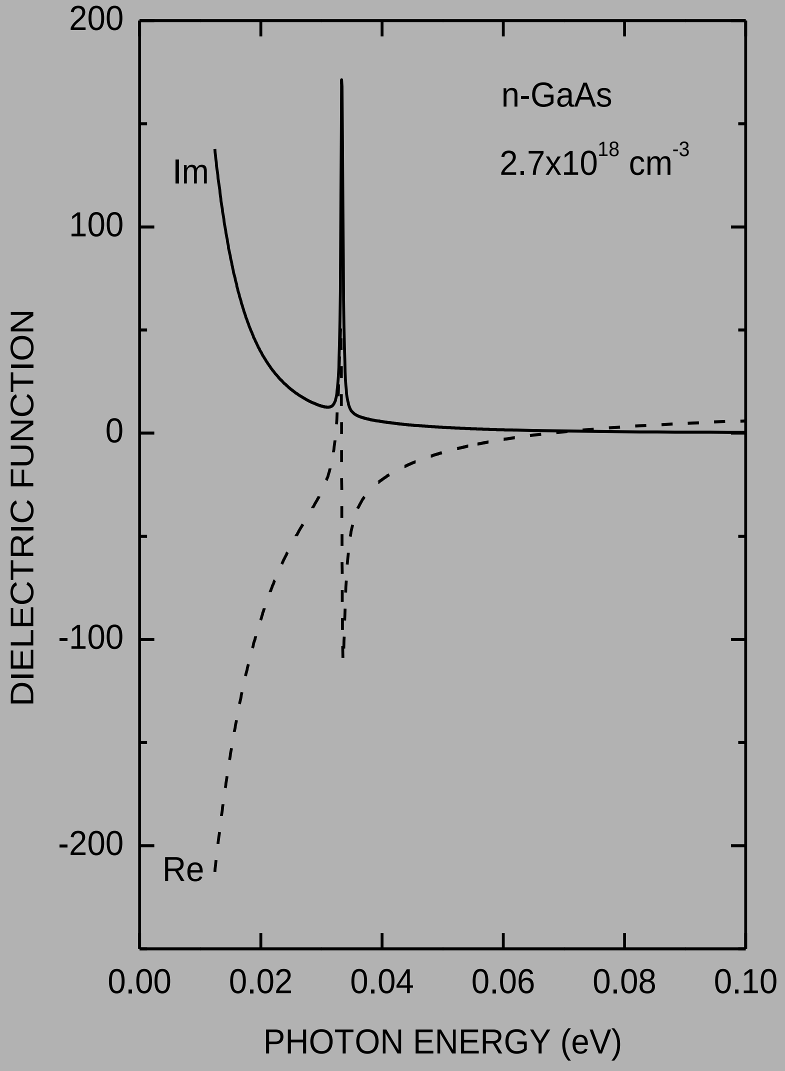
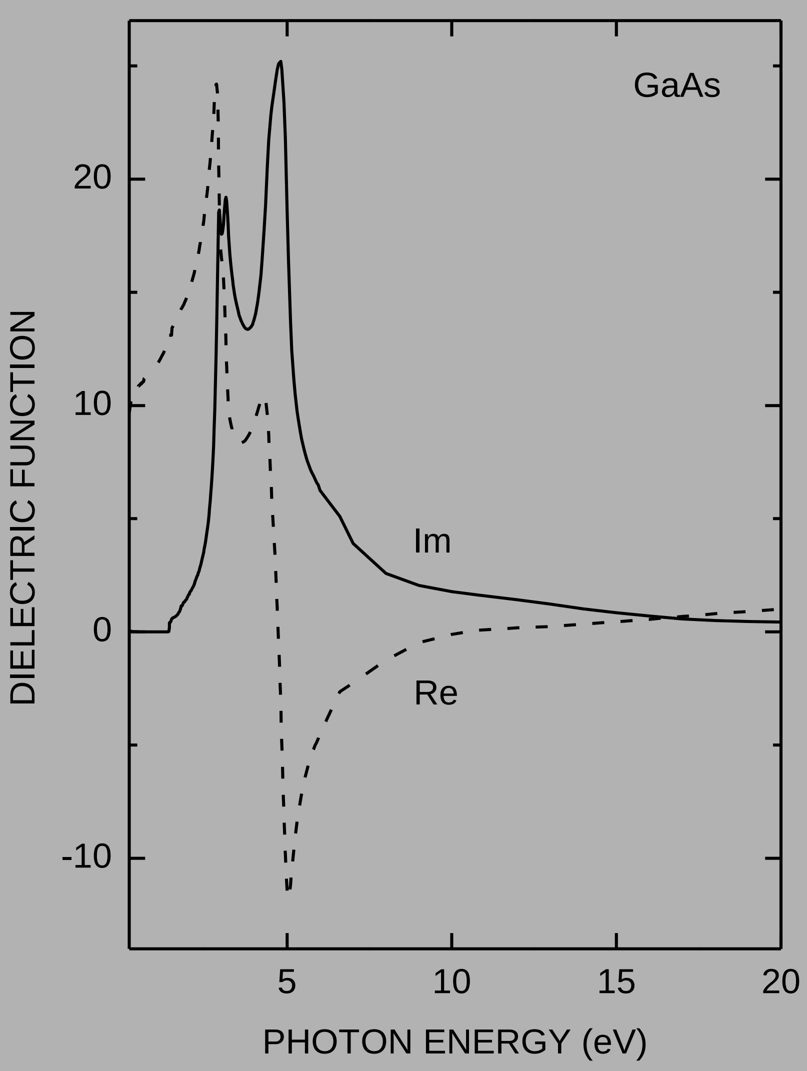


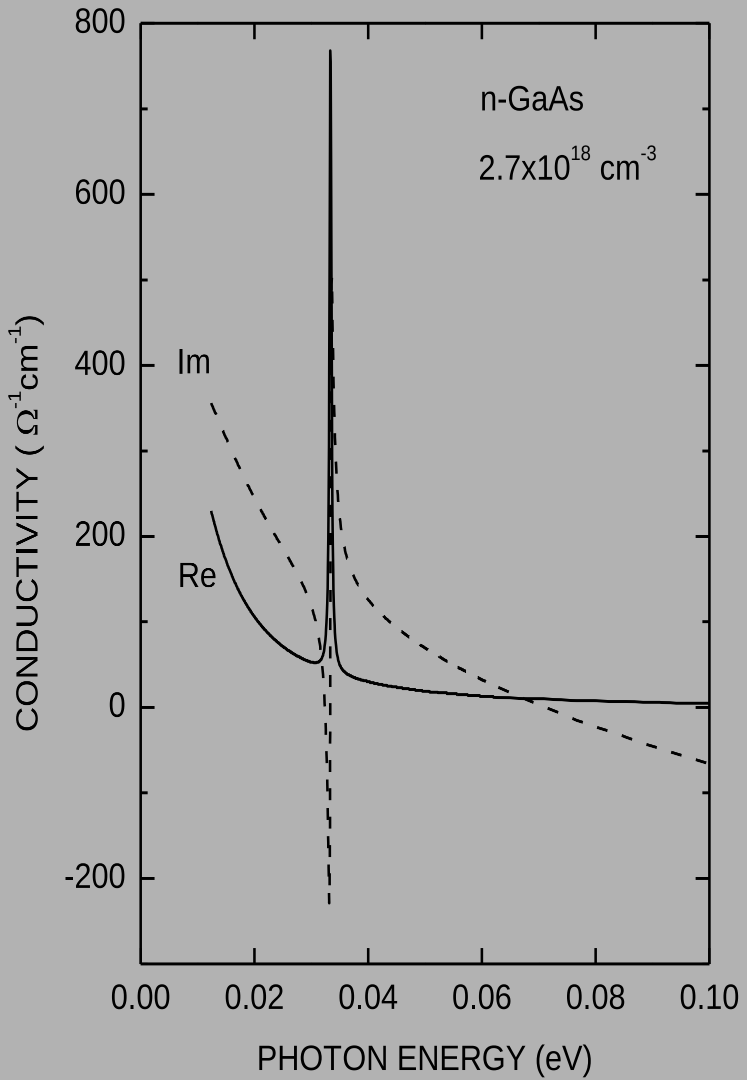
Fig. 8.29. Valence band charge density for gallium arsenide. The charge density contours are in units of electrons per unit cell volume

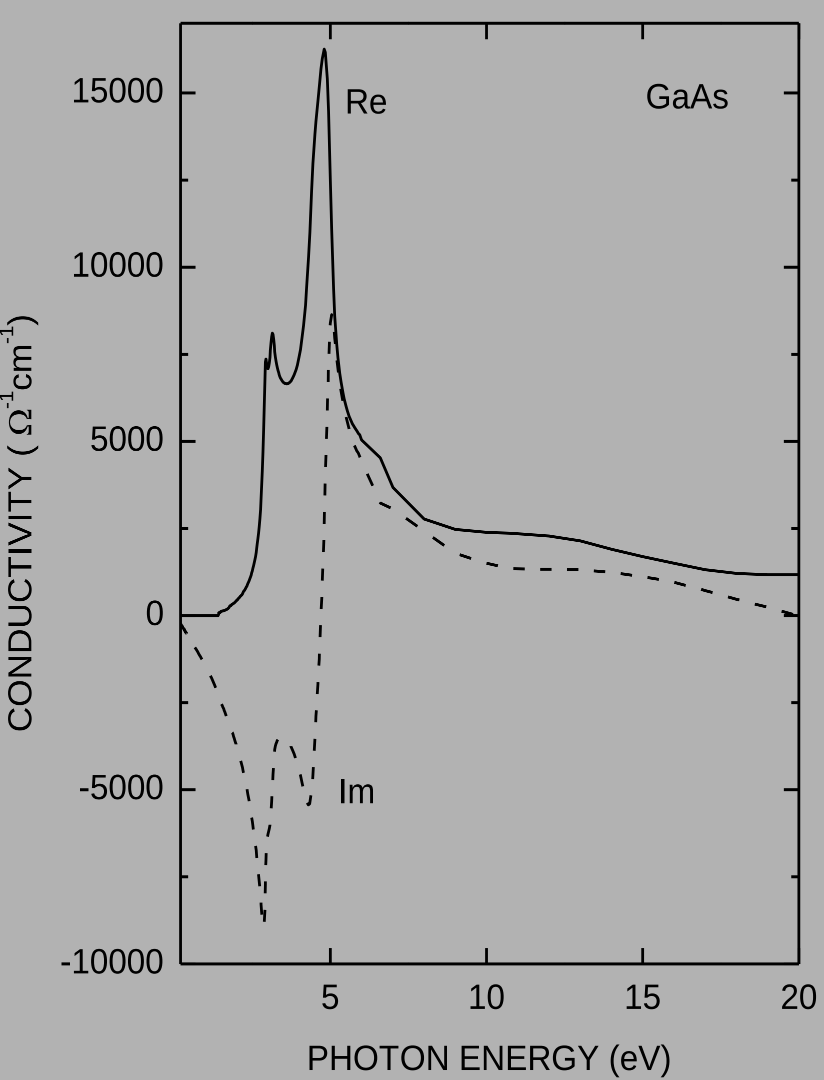
Doped GaAs – dielectric function



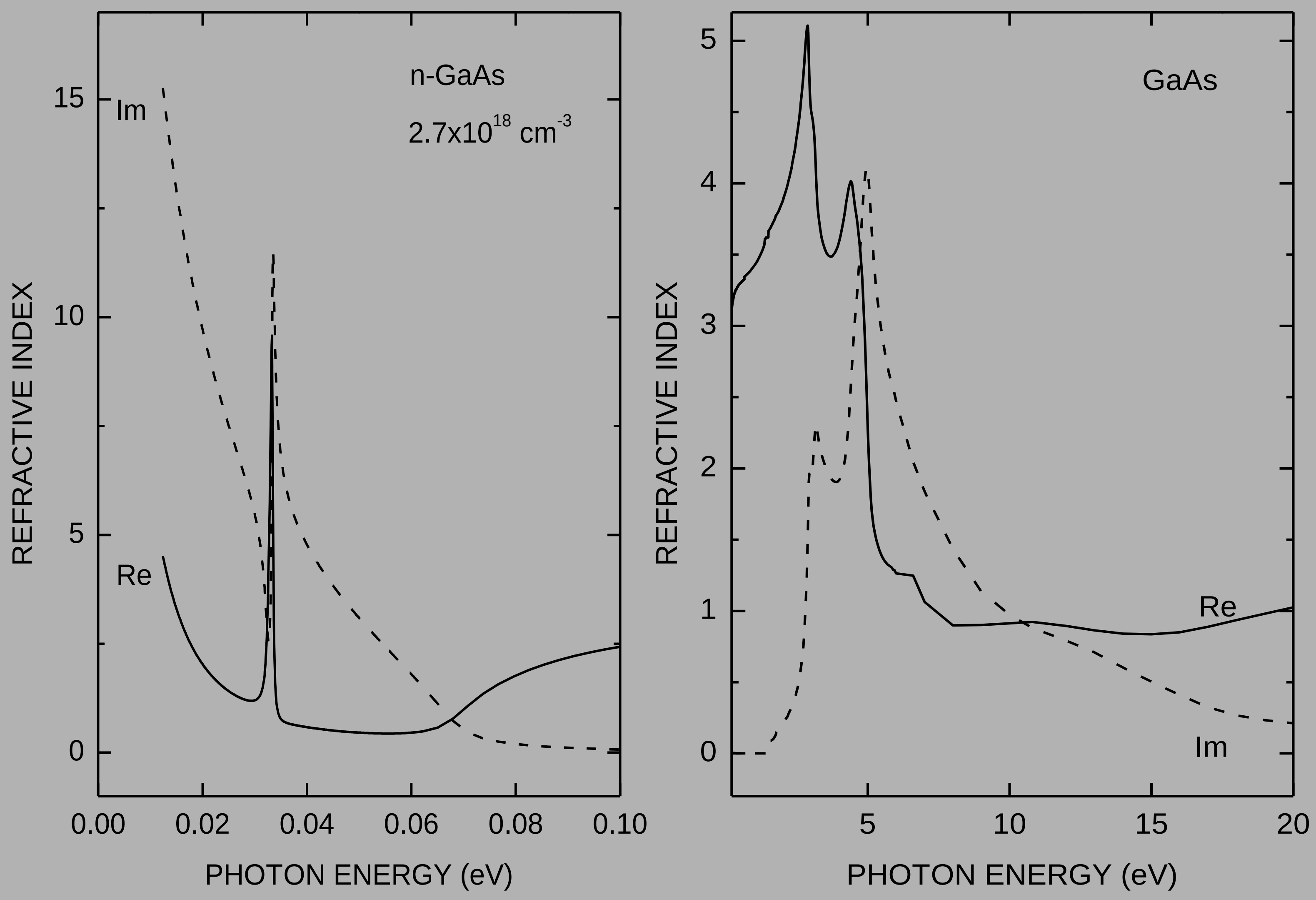


Doped GaAs - conductivity

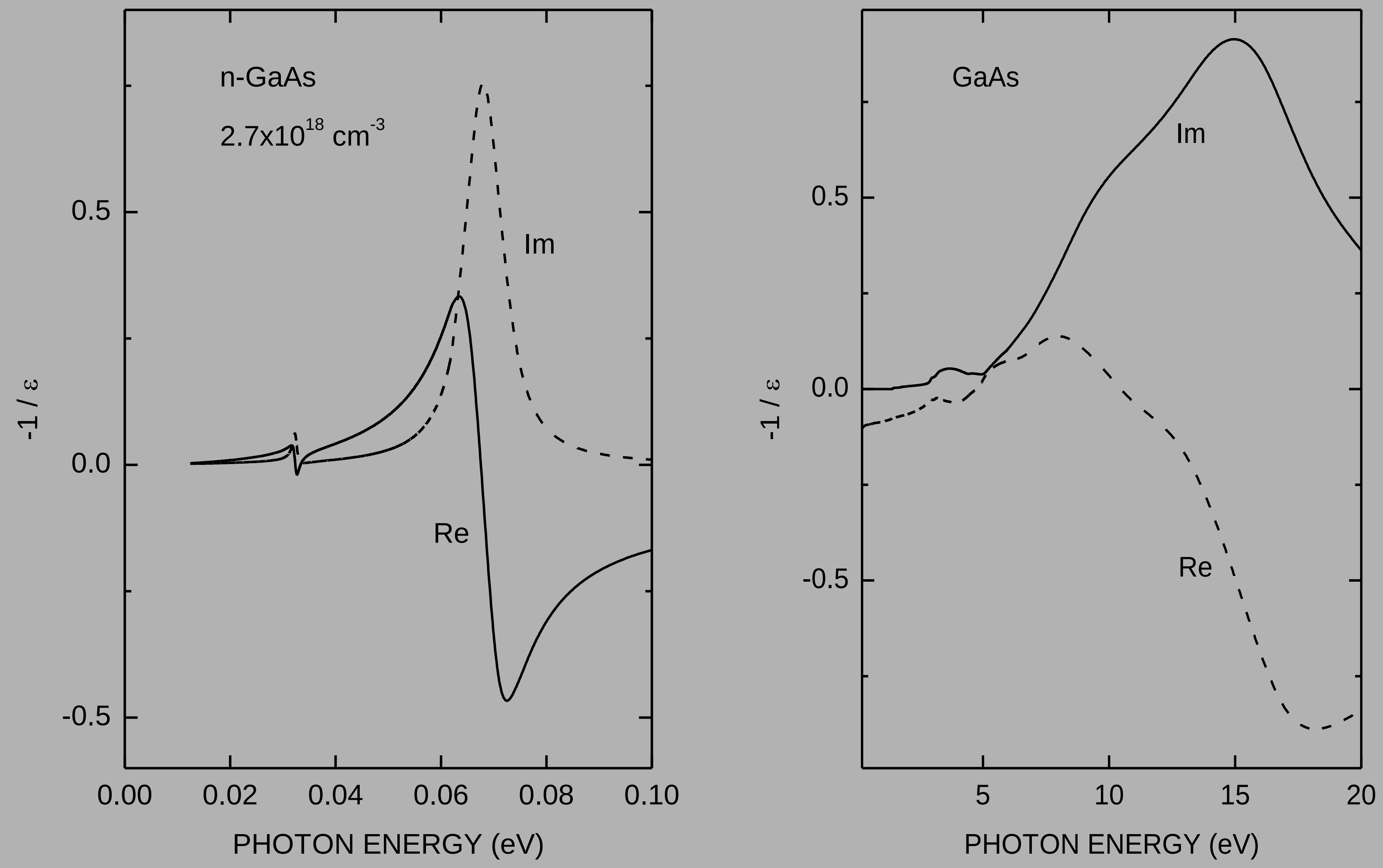




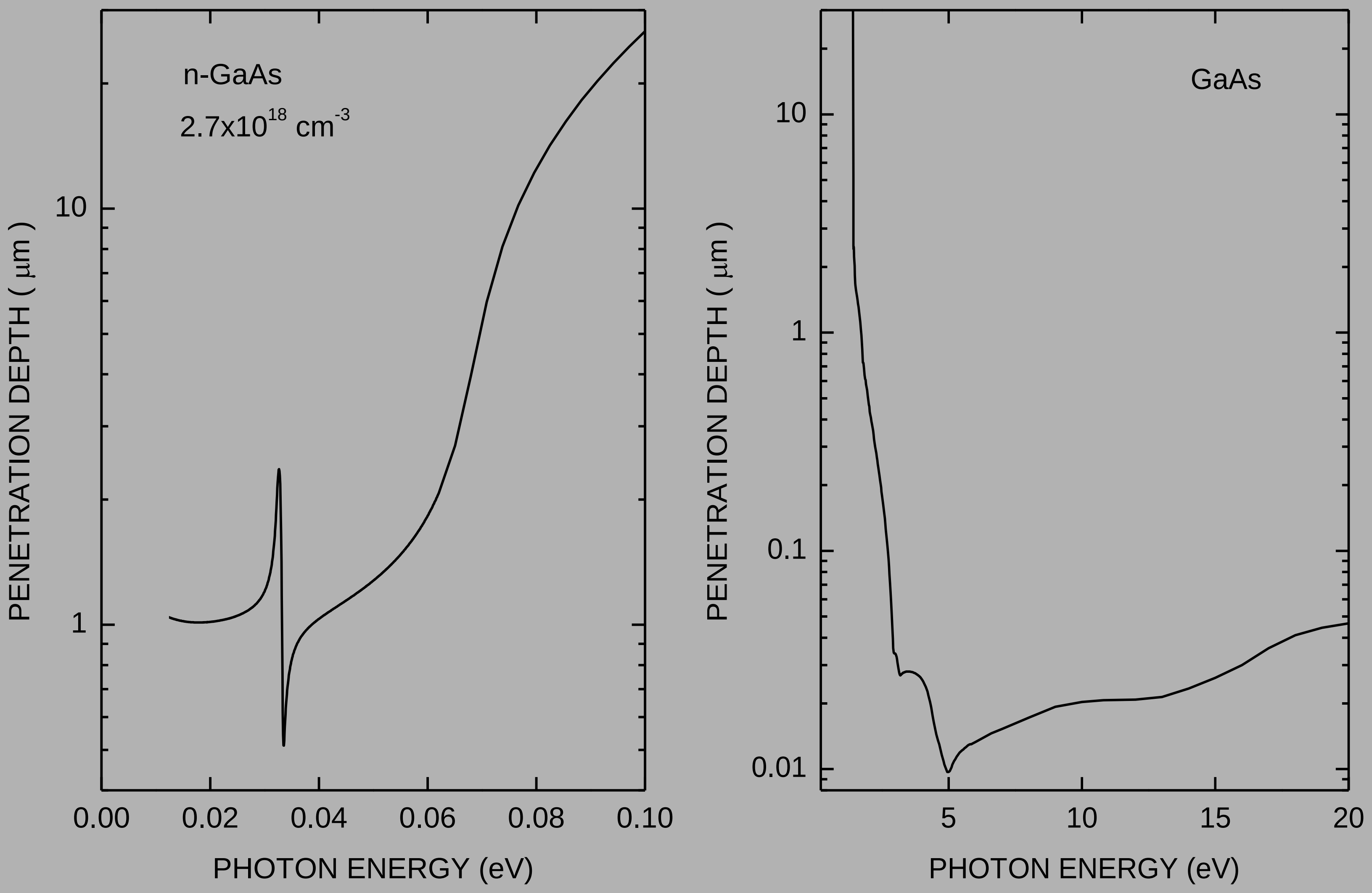
Doped GaAs – refractive index



Doped GaAs – inverse dielectric function



Doped GaAs – penetration depth



Doped GaAs – normal-incidence reflectivity