



The shift in the optical band-gap of cadmium oxide as chemical potential minus optical potential



M.A. Grado-Caffaro^{*,1}, M. Grado-Caffaro

Scientific Consultants, C/ Julio Palacios 11, 9-B, 28029 Madrid, Spain¹

ARTICLE INFO

Article history:

Received 7 November 2014

In final form 21 January 2015

Available online 29 January 2015

ABSTRACT

The shift in the band-gap experienced by CdO is treated theoretically as approximately the chemical potential minus the optical potential. These potentials are assumed to be dependent on the partial pressure of oxygen in the cadmium deposition process since the shift depends on this pressure. We obtain an approximate relationship for the electron–hole scattering length from that (which is established here as main result) the chemical potential is roughly null when the CdO electron concentration is maximum, which (as we will show) is equivalent to say that the chemical potential becomes approximately zero if the optical transmittance in CdO is maximal.

© 2015 Elsevier B.V. All rights reserved.

1. Introduction

Nowadays, the role played by cadmium oxide is well-known as very transparent (in the visible range) semiconductor. Certainly, as other transparent conducting and semiconducting oxides, CdO thin films have a number of applications in optoelectronics and, for example, for electroplating baths, electrodes for storage batteries, and ceramic glazes. Perhaps the most known application of CdO is as transparent contact in solar cells and as antireflection coating. On the other hand, we have to mention that this oxide has been investigated experimentally with quite satisfactory results [1–12] and by elaborating successfully theoretical–analytical approaches [13–17]. But, unfortunately, some works as, for instance, Refs. [18,19] were clearly erroneous. The shift in the optical band-gap exhibited by some oxides as, for example, CdO, known in the current literature as the Burstein–Moss effect, is directly related to the subject of the present letter. At room temperature, an energy band-gap shift from 2.3 eV to 2.7 eV was measured in cadmium oxide [3] while a shift from 2.40 eV to 2.42 eV was observed [4] as well as from 2.32 eV up to 2.52 eV [1]. The aforementioned shift varies with the partial pressure of oxygen relative to the growth of CdO crystals and also changes with temperature.

The partial pressure of oxygen during the deposition process of cadmium oxide is a key issue in the context of the present letter. It is well-known that the electrical and optical properties of CdO depend

strongly on the aforementioned pressure (see, for instance, Refs. [1,2]). In particular, the dependence on this pressure of the CdO band-gap shift is really notorious. As a matter of fact, in this letter, we shall treat (theoretically) the shift in the optical energy band-gap of CdO by means of a, say, very special model. In this model, the role of the partial pressure of oxygen acquires a great importance. We will tackle the shift in question as the approximate difference between the corresponding chemical-potential energy and optical-potential energy. In this treatment, the concept of optical potential arises. This concept, coming from the many-body problem, is really very significant in several branches of Physics [20–29] as, for instance, nuclear astrophysics, Bose condensation, superfluidity, and superconductivity, but not much has been done upon it. In particular, the notion of optical potential is manifestly relevant in Condensed Matter Physics (consider, for example, superconductivity in solids). Here we will use this concept with success providing an elegant formulation on the basis of envisaging CdO thin films as dilute degenerate Fermi gases. In this context, on the basis that zero chemical potential means that the spatial electron density is maximum (a fact which we will prove), we will find an approximate formula for the electron–hole scattering length. In addition, we will show that, in a first approximation, the above maximum value corresponds to maximum optical transmittance in the visible range.

2. Theoretical formulation

The chemical-potential energy of a degenerate dilute Fermi gas reads $\mu \approx E_F + V$ where E_F denotes Fermi energy and V stands for optical-potential energy (see, for instance, Refs. [21,25–28]). On the

* Corresponding author.

E-mail address: ma.grado-caffaro@sapienzastudies.com (M.A. Grado-Caffaro).

¹ www.sapienzastudies.com.

other hand, it is well-known that the shift in the optical band-gap of cadmium oxide (which always is n-type) coincides with its Fermi energy so this shift, for low absolute temperature, reads within the quasi-free electron theory:

$$\Delta E_g(P) = \frac{\hbar^2}{2m_r^*} [3\pi^2 n(P)]^{2/3} \quad (1)$$

where \hbar is the reduced Planck constant, P denotes partial pressure of oxygen, m_r^* is electron–hole reduced effective mass, and $n(P)$ stands for electron spatial density.

Expression (1) represents the Burstein–Moss effect by which the apparent band-gap of CdO (a degenerate semiconductor) is increased as the absorption edge is pushed to higher energies as a consequence of the fact that all states near the conduction band are populated (the electron density is larger than the effective density of states at the conduction-band edge). The effect in question is enhanced if donor impurities are added to CdO. In this respect, we wish to note that, in nominally doped semiconductors, the Fermi level lies between the conduction and valence bands. As the donor density in CdO is increased, then electrons populate states within the conduction band, pushing the Fermi level higher in energy. As a matter of fact, the Fermi level lies in the conduction band if a given (degenerate) semiconductor is n-type as, for example, cadmium oxide. All the states below the Fermi level are occupied and excitation into these occupied states cannot occur by virtue of the exclusion principle. The apparent band-gap equals the actual band-gap plus the Burstein–Moss shift (see, for instance, Ref. [30]) so, considering an optical transition, it is clear that the minimum photon energy must be almost equal to the band-gap energy plus the above shift given that the effective electron mass is much smaller than the effective hole one [30].

At low absolute temperature, the corresponding optical-potential energy is:

$$V(P) = \frac{2\pi\hbar^2 b n(P)}{m_r^*} \quad (2)$$

where b (which here is constant) designates electron–hole scattering length. Given that, of course, the Coulomb electron–hole interaction is attractive, then we have that $b < 0$ (attractive optical potential).

Eq. (2) arises from the original expression namely $V = 2\pi\hbar^2 b n/m$ where m stands for neutron rest-mass. This last expression corresponds, in reality, to a pseudo-potential energy relative to neutron–nucleus interaction [20–29], V and n being functions of spatial coordinates; generalizing, m is fermion rest-mass. Since $b < 0$, then $V < 0$; let us assume that the integral of V over its spatial domain is finite. By the definition of μ and formulas (1) and (2), then we have that $\mu \approx Cn^{2/3} - |b|n$ (dilute degenerate gas), where C is a non-negative constant. From this last formula, it follows that $\mu \rightarrow -\infty$ as $n \rightarrow \infty$, that is, the gas collapses [28]. On the other hand, the expression namely $V = 2\pi\hbar^2 b n/m$ becomes formula (2) through a transformation of spatial-coordinate space into P -space. Formula (2) is applicable to non-relativistic (attractive or repulsive) neutron–neutron scattering [21,25–28] as well as electron–nuclei scattering. In the context of neutron–neutron scattering, optical potential and refractive index may be derived from the so-called Born forward scattering amplitude [21,23–28]. On the other hand, the scattering length (or amplitude) b may be obtained from concrete equations and can have a sign different than the Born length [21,23–28] so that this difference is really very important to fix the sign of the optical potential [21,23–28]. To exemplify, we can mention that neutron–neutron scattering gives rise to large attractive optical potential in a neutron star, which compresses the star together with gravitational field [21,23–28]. Within this framework, one regards a neutron gas as a collection of identical particles which exert a pressure, this pressure being a relevant physical

Table 1
CdO electron concentration versus P .

P (Torr)	n (10^{19} cm^{-3})
1×10^{-4}	7.3
5×10^{-4}	12.5
1×10^{-3}	12.7
5×10^{-3}	11.3
1×10^{-2}	2.0

quantity. As a result, by the exclusion principle, repulsive interaction counteracting gravity takes place [21,23–28].

Returning now to Eq. (2), we emphasize that we refer to electron–hole scattering, which is somewhat similar to electron–atom scattering (see Refs. [20–29]). Making $b \equiv -|b|$ into expression (2), it is not hard to see that the chemical-potential energy of degenerate CdO as a dilute Fermi gas tends to vanish as $n(P)$ attains its maximum value. From this fact, taking into account formulas (1) and (2), and making into Eq. (1) the approximation $(3\pi^2)^{2/3} \approx (\pi^3)^{2/3} = \pi^2$, then it follows:

$$|b| \approx \frac{\pi}{4} [n(P_0)]^{-1/3} \quad (3)$$

where P_0 is the value of P at which the function $n(P)$ achieves its maximum value which, of course, is $n(P_0)$.

From Ref. [1], Fig. 2, one has that $n(P_0) \approx 12.7 \times 10^{19} \text{ cm}^{-3}$, which replaced into (3), yields $|b| \approx 1.5 \text{ nm}$. In Table 1, we have collected significant values of $n(P)$ extracted from Ref. [1], Fig. 2.

One has that $P_0 \approx 1 \times 10^{-3} \text{ Torr}$, this value being the so-called optimum partial pressure of oxygen at which the optical transmittance (in the visible region) of CdO is maximum achieving 90% (see Table 2). As a matter of fact, in Table 2, some experimental values of transmittance (depending on the partial pressure of oxygen and denoted by T) in the visible range are given (after Ref. [1]).

We emphasize that from Ref. [1], Fig. 2, it follows that, approximately, the electron spatial density attains its maximal value at the optimum oxygen partial pressure (notice that Fig. 2 of Ref. [1] is referred to logarithmic scale). Consequently, as we have said earlier, zero chemical potential implies (roughly) maximum optical transmittance in the visible range. On the other hand, by inserting (3) into (2) and considering expression (1), we get:

$$\Delta E_g(P_0) \approx \frac{h^2}{8m_r^*} [n(P_0)]^{2/3} \quad (4)$$

where of course, $h = 2\pi\hbar$.

Another interesting issue to be treated is related to regarding the finite-increment formula:

$$\Delta E_g = \left[\frac{dE_g(P)}{dP} \right]_{P=P_0} \Delta P \quad (5)$$

In order to equate (1) with (5), it is clear that the left-hand side of (1) becomes ΔE_g instead of the initial $\Delta E_g(P)$ so P on the right-hand side of (1) becomes a fixed value which, by convenience, is P_0 . Also, we take $\Delta P = P_1 - P_2$ such that $P_2 < P_0 < P_1$. Then, by equating (1) with (5), one can obtain the first derivative of $E_g(P)$ at P_0 in terms

Table 2
CdO visible-range transmittance versus P (after Ref. [1]).

P (Torr)	T (%)
2×10^{-4}	85
1×10^{-3}	90
5×10^{-3}	80
1×10^{-2}	75

Download English Version:

<https://daneshyari.com/en/article/5380115>

Download Persian Version:

<https://daneshyari.com/article/5380115>

[Daneshyari.com](https://daneshyari.com)