

A MATHEMATICAL FORMULATION FOR DIAMAGNETISM IN TETRAHEDRALLY BONDED SEMICONDUCTORS

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An expression for the magnetic susceptibility tensor corresponding to diamagnetic contribution in tetrahedrally bonded semiconductors is derived; this formulation refers to the crystalline state. In addition, a comparison with the amorphous case is outlined.

INTRODUCTION

A mathematical formulation for the magnetic susceptibility of a typical tetrahedrally bonded amorphous semiconductor has recently been performed [1]. Since an amorphous solid is isotropic, the magnetic susceptibility tensor may be expressed as $\bar{\chi} = \chi \bar{1}$. Therefore, we have $\chi_{xx} = \chi_{yy} = \chi_{zz}$ and since $\bar{\chi} = \bar{\chi}^{(p)} + \bar{\chi}^{(d)}$, where (p) denotes paramagnetic and (d) diamagnetic, we can write $\chi_{xx}^{(d)} = \chi_{yy}^{(d)} = \chi_{zz}^{(d)}$. In the following, we will expose a formulation for the diamagnetic term of the susceptibility of a typical tetrahedral semiconductor in the crystalline state; since this state implies anisotropy, we have $\chi_{xx} \neq \chi_{yy} \neq \chi_{zz}$ so that $\chi_{xx}^{(d)} \neq \chi_{yy}^{(d)} \neq \chi_{zz}^{(d)}$. The formulation in question is based on linear response theory and the Wannier model. On the other hand, it is well-known that in the amorphous state, disorder gives rise to a reduced paramagnetic contribution so that a net enhancement of diamagnetism takes place; this does not occur in the crystalline state.

THEORY

Assume a system with an eigenvalue spectrum formed by two bands so that [1]:

$$\hat{H}|\psi_{nn'}\rangle = E_{nn'}|\psi_{nn'}\rangle \quad (1)$$

where \hat{H} denotes hamiltonian, n is the band index ($n = 0$ or 1), and n' denotes the states in the bands; eq. (1) is of course the time-independent Schrödinger equation. On the other hand, we assume that the ground state of the system is such that all the states in the $n = 0$ band are filled. Now we state:

$$\bar{\chi} \equiv \begin{pmatrix} \chi_{xx} & 0 & 0 \\ 0 & \chi_{yy} & 0 \\ 0 & 0 & \chi_{zz} \end{pmatrix} \quad (2)$$

so that:

$$\bar{\chi}^{(d)} \equiv \begin{pmatrix} \chi_{xx}^{(d)} & 0 & 0 \\ 0 & \chi_{yy}^{(d)} & 0 \\ 0 & 0 & \chi_{zz}^{(d)} \end{pmatrix} \quad (3)$$

by taking into account that the situation in which $\chi_{xy}^{(p)} + \chi_{xy}^{(d)} = 0$, $\chi_{yz}^{(p)} + \chi_{yz}^{(d)} = 0$ and $\chi_{xz}^{(p)} + \chi_{xz}^{(d)} = 0$ is meaningless. We establish:

$$\chi_{xx}^{(d)} = -\alpha \sum_i \langle \psi_{oi} | y^2 + z^2 | \psi_{oi} \rangle \quad (4)$$

$$\chi_{yy}^{(d)} = -\beta \sum_i \langle \psi_{oi} | x^2 + z^2 | \psi_{oi} \rangle \quad (5)$$

$$\chi_{zz}^{(d)} = -\gamma \sum_i \langle \psi_{oi} | x^2 + y^2 | \psi_{oi} \rangle \quad (6)$$

where α , β and γ are real constants ($\alpha > 0$, $\beta > 0$, $\gamma > 0$). Note that the wave-function $\psi_{oi}(x, y, z)$ fulfills eq. (1) so that $\hat{H}|\psi_{oi}\rangle = E_{oi}|\psi_{oi}\rangle$. From (4), (5), and (6), it is deduced that

$$\chi_{xx}^{(d)} = -\alpha \iiint_D (y^2 + z^2) \left[\sum_i |\psi_{oi}(x, y, z)|^2 \right] dx dy dz \quad (7)$$

$$\chi_{yy}^{(d)} = -\beta \iiint_D (x^2 + z^2) \left[\sum_i |\psi_{oi}(x, y, z)|^2 \right] dx dy dz \quad (8)$$

$$\chi_{zz}^{(d)} = -\gamma \iiint_D (x^2 + y^2) \left[\sum_i |\psi_{oi}(x, y, z)|^2 \right] dx dy dz \quad (9)$$

where D is the spatial domain corresponding to the semiconductor sample considered. Eqs. (7), (8) and (9) constitutes a set of explicit formulae that becomes useful for numerical calculations.

DISCUSSION

In certain cases [1], for disordered states we have $\chi_{xx}^{(d)} = \chi_{yy}^{(d)} = 0$, $\chi_{zz}^{(d)} \neq 0$; however, for the crystalline counterpart we have the preceding expressions. These formulae have been established from linear response theory and a Wannier representation. Our formulation is related to theoretical work on electron-spin resonance and associated problems developed in refs. [2] [3] [4]; this work refers to amorphous semiconductors. It is well-known that the tensor of electron-spin resonance is the g

tensor; this tensor is related to singly occupied dangling bond states. These states can be considered as deep levels in the gap of amorphous silicon because of three-fold coordinated Si atoms [4] [5].

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