Active and Passive Elec. Comp., 1995, Vol. 17, pp. 253–255
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MAGNETIC SUSCEPTIBILITY OF TETRAHEDRALLY BONDED AMORPHOUS SEMICONDUCTORS

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(Received August 5, 1994; in final form September 7, 1994)

A special theoretical formulation on the magnetic susceptibility of tetrahedral amorphous semiconductors is proposed. This formulation is based upon a Wannier representation involving two terms: a diamagnetic term and a paramagnetic contribution. In addition, electron-spin resonance referred to amorphous silicon is considered.

1. INTRODUCTION

Electron-spin resonance in amorphous Si has been studied by a large number of authors. In particular, we can mention experimental work realized by S.C. Moss and J.F. Graczyk,[1] M.H. Brodsky and R.S. Title,[2] P.A. Thomas et al.,[3] etc. On the other hand, recent theoretical work by M. Stutzmann and D.K. Biegelsen,[4] S. Yamasaki et al.,[5] and M.A. Grado and M. Grado[6] has been developed. In ref. [6], magnetic susceptibility has been investigated with respect to the tensor of electron-spin resonance (g tensor).

The aim of the present work consists of a clarification of the basic theory corresponding to the enhanced diamagnetism of tetrahedral amorphous semiconductors. This clarification will be realized by introducing a new formulation based upon a Wannier representation. Moreover, this model will include considerations related to the g tensor. This tensor plays an important role in the context of singly occupied dangling bond states. In refs. [2] and [6], these states are regarded as deep levels in the gap of amorphous Si because of three-fold coordinated Si atoms.

2. THEORY

Let us start by supposing that we refer to a system with an eigenvalue spectrum formed by two bands so that:

$$\hat{H}|nn'\rangle = E_{nn'}|nn'\rangle \tag{1}$$

where $\hat{H}$ denotes hamiltonian operator, E means energy, n stands for the band index (n = 0 or 1), and n′ denotes the states in the bands. The ground state of the system is such that all the states in the n = 0 band are filled. Following ref. [7] we have:

$$\chi_{zz} = -\frac{m}{2} \sum_{i} \langle 0i|x^2 + y^2|0i\rangle + \sum_{i,j} \langle 0i|\hat{L}_z|1j\rangle\langle 1j|\hat{L}_z|0i\rangle \, (E_{1j} - E_{0i})^{-1} \qquad (2)$$

where χ_{zz} is the zz-component of the magnetic susceptibility tensor:

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

On the other hand, $\hat{L}_z$ is the angular momentum operator. The first term of the right-hand side of eq. (2) is diamagnetic, and the second term is paramagnetic; this positive-definite term can be expressed by means of a dyadic product of matrices, as follows:[8]

$$\chi_{zz}^{(p)} = \mathrm{tr}(\zeta_{ij} \otimes \xi_{ij}) \qquad (3)$$

where tr denotes trace and:

$\zeta_{ij} \equiv \langle 0i|\hat{L}_z|1j\rangle\langle 1j|\hat{L}_z|0i\rangle \equiv |\langle 0i|\hat{L}_z|1j\rangle|^2$

$\xi_{ij} \equiv (E_{1j} - E_{0i})^{-1}$

Finally, we have deduced:

$$\langle 0i|\hat{L}_z|1j\rangle\xi_{ij} \approx c \int_0^\infty \langle 0i|e^{\lambda\hat{H}}\hat{L}_z e^{-\lambda\hat{H}}|1j\rangle d\lambda \qquad (4)$$

where c is a constant. Eq. (4) is consistent with ref. [7].

3. DISCUSSION

We have found a special tensorial representation for the paramagnetic term of χ_{zz} in tetrahedral amorphous semiconductors. In addition, we have introduced an integral representation that becomes useful to study the magnetic properties of amorphous silicon. The diamagnetic term has also been considered. In reality a diamagnetic enhancement takes place. Finally, we want to remark that electron-spin resonance is related to the free spin density and the diamagnetic enhancement. In particular, evaporated amorphous semiconductors exhibit a free spin density that depends strongly upon annealing temperature.

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