ELECTRONIC PROPERTIES AND DYNAMIC SUSCEPTIBILITY OF MnTe SYSTEMS

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Thin MnTe films are investigated. Electronic structure, local density of states and local magnetic moments are calculated for systems with ferromagnetic and antiferromagnetic order. Spin-dependent modifications of the density of states near the surface are results of the changes in p–d hybridization. Magnetic longitudinal and dielectric susceptibilities are calculated.

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Properties of MnTe, CdMnTe systems and especially (Cd)MnTe/CdTe quantum wells have been investigated by using various experimental techniques. Theoretical investigations concerning the band structure calculations were performed mainly for hypothetical MnTe crystals with zinc blende structure as well as for mixed CdMnTe bulk systems (e.g. [1, 2]). Problems of electronic structure and magnetic properties of ultrathin films are undertaken in the paper.

Films consisting of 10 MnTe layers with free surfaces of (110) and (100) types are considered. Calculations are performed within the framework of the tight-binding approach. Atomic orbitals of d and s symmetry are taken as basis functions for Mn ions, whereas p states are chosen for Te ions. p–d hybridization which plays the crucial role in MnTe systems [2] is strictly taken into account. The Slater–Koster parameterization is used. Hoppings between the nearest and the next-nearest neighbours are taken into account. Values of parameters are adjusted in such a way that the main features of the electronic structure characteristic of bulk materials are reproduced in our calculations for bulk MnTe. The splitting of d-bands is assumed to be 7 eV in consistency with experimental data [3]. Calculations are performed for MnTe films with hypothetical ferromagnetic (F) and antiferromagnetic (AFI) order. In the last case the moments are ordered ferromagnetically in planes, but couplings between neighbouring layers are antiferromagnetic.

Electronic band structure, local density of states and local magnetic moments are calculated for systems under investigations. Partial densities of states for cations and anions are also found. The obtained results are depicted in Fig. 1. The density of states for the central plane resembles well the one characteristic of
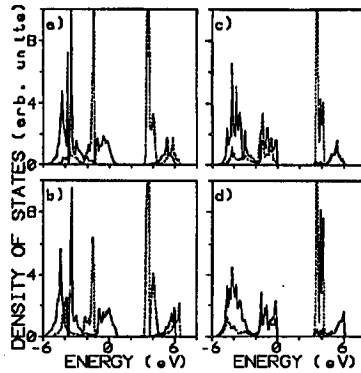
Fig. 1. Total density of states calculated for MnTe (110) films in the (a) surface and (b) central layer with F order, (c) surface and (d) central layer with AFI order. Full and dashed lines correspond to majority and minority spin, respectively.

bulk material. Positions of main peaks corresponding to Mn agree well with known results [3].

Films with free surfaces are investigated. In fact it is difficult to find reliable data on a reconstruction or relaxation in these materials. States localized near the surface lying mainly in the valence band are found. The surface density of Mn states is enhanced and a small enhancement of the magnetic moment of Mn ions is observed. The surface perturbation is well localized in the surface layer and only small changes take place in the density of states for subsurface plane.

A negative splitting of the valence band edge is found in all layers for films with F order. Calculations performed for films with AFI couplings between layers show that for inner planes there is no splitting of the edge of the valence band and the density of states corresponding to Te ions in the central layer is practically independent of the spin direction. Spin dependent changes are found in the surface density of Te states. The modifications are results of the changes in p–d hybridization. The exchange fields do not fully compensate near the surface because of the reduced number of neighbouring magnetic ions.

The calculated results are used in investigations of the dynamic susceptibility. In magnetic systems the longitudinal magnetic and dielectric susceptibilities are strongly coupled [4]. Both types of the susceptibility (magnetic and dielectric) are determined by the function $\Gamma_\sigma(\omega, q)$, which is the so-called non-enhanced susceptibility [4, 5]. For bulk crystals within the framework of the Hubbard model the longitudinal susceptibility can be expressed in a simple form [4, 5]

$$\chi_{\sigma\sigma} = \frac{\Gamma_\sigma + \Gamma_{-\sigma} + 2V\Gamma_\sigma\Gamma_{-\sigma}}{1 - V^2\Gamma_\sigma\Gamma_{-\sigma}}, \tag{1}$$

where V represents the electron–electron interaction and σ corresponds to spin. The main features of Γ can be in fact represented by a joint density of states. In the case of thin films more complicated matrix equation can be obtained [6]. However, in films the susceptibility is also determined by the non-enhanced Γ function which depends in this case on the layer index.
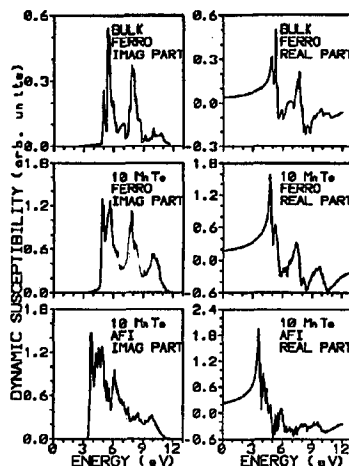
Fig. 2. The dynamic susceptibility for bulk F MnTe and for the central plane of MnTe (110) films with F and AFI order.

Real and imaginary parts of $\Gamma_\sigma(\omega, q)$ are calculated for bulk systems and thin films. It is found that in systems with F order the product of $\Gamma_\sigma \Gamma_{-\sigma}$ is small in comparison to $\Gamma_\sigma + \Gamma_{-\sigma}$ in the whole energy region. Therefore, there is practically no enhancement (Eq. (1)) and both magnetic and dielectric susceptibilities are directly determined by Γ_σ. In AFI case an enhancement is obtained at low energies, however, a strong damping appears in the high energy region. The calculated magnetic susceptibility is depicted in Fig. 2. A presence of Mn d states essentially influences the susceptibility leading to high peaks. The first peak in imaginary part corresponds to transitions between valence $p_\downarrow$ states and unoccupied $d_\downarrow$ states, mainly with e_g symmetry at L point in the Brillouin zone. Optical transitions of this type are observed in CdMnTe systems [3].

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