Properties of MgB_2 in a two-gap superconductivity model

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Abstract

For MgB_2 where coexist two coupled superconductivity gaps a two-band scheme has been developed. Three interaction channels have been taken into account: a pair-transfer type $\sigma-\pi$-interband repulsion, a σ-intraband effective attraction of electron-phonon nature, and a σ-intraband Coulomb interaction. The calculated temperature dependencies of gaps, heat capacity and H_{c2} agree with the experimental findings. The theoretical curve of T_c *vs* x for $Mg_{1-x}Al_xB_2$ follows the experimental data.

Key words:
MgB_2; two-band model; superconductivity and thermodynamic characteristics

A number of experiments point to the two-gap nature of the MgB_2 superconductivity [1-6]. The electron structure calculations [7,8] also support this conclusion by revealing the Fermi level intersection by boron σ- and π-bands. At the same time, there is no doubt in the presence of strong σ-intraband pairing interaction in MgB_2 [7,8], however, the mentioned circumstances suggest to introduce the interband pairing channels and the use of two-band models of superconductivity [5,9-12].

The linearized Hamiltonian of the system incorporating electron-phonon and Coulomb interactions in the effective σ-band, and the $\sigma-\pi$ scattering of intraband pairs is taken in the form

$$H=\sum_{\alpha\mathbf{k}s}\tilde{\epsilon}_\alpha(\mathbf{k})a^+_{\alpha\mathbf{k}s}a_{\alpha\mathbf{k}s}-\sum_{\alpha\mathbf{k}}\triangle_{\alpha\mathbf{k}}<a^+_{\alpha\mathbf{k}\uparrow}a^+_{\alpha-\mathbf{k}\downarrow}> +\sum_{\alpha\mathbf{k}}(\triangle_{\alpha\mathbf{k}}a^+_{\alpha\mathbf{k}\uparrow}a^+_{\alpha-\mathbf{k}\downarrow}+\triangle^*_{\alpha\mathbf{k}}a_{\alpha-\mathbf{k}\downarrow}a_{\alpha\mathbf{k}\uparrow}), \quad (1)$$

where the superconductivity order parameters are defined as $\triangle_{\alpha\mathbf{k}}=2\sum_{\beta\mathbf{k}'}W_{\alpha\beta}(\mathbf{k},\mathbf{k}')<a_{\beta-\mathbf{k}'\downarrow}a_{\beta\mathbf{k}'\uparrow}>$. The band energies ($\alpha=1$ for σ and $\alpha=2$ for π) read $\epsilon_\alpha=\tilde{\epsilon}_\alpha+\mu$, where μ is the chemical potential. Other common designations are used. The gap equations ($\Theta=k_BT$)

$$\triangle_{\alpha\mathbf{k}}=-\sum_{\beta\mathbf{k}'}W_{\alpha\beta}(\mathbf{k},\mathbf{k}')\triangle_{\beta\mathbf{k}'}\xi_{\beta\mathbf{k}'} \quad (2)$$

with $\xi_{\alpha\mathbf{k}}=E^{-1}_\alpha(\mathbf{k})\tanh[E_\alpha(\mathbf{k})/2\Theta]$ contain the quasiparticle energies $E_\alpha(\mathbf{k})=[\tilde{\epsilon}^2_\alpha(\mathbf{k})+\triangle^2_{\alpha\mathbf{k}}]^{1/2}$. The gaps are taken to be real.

Describing the s-wave superconductivity of MgB_2 the σ-intraband coupling constant $W_{11}=V+U$ is supposed to contain a Coulombic part $U>0$ besides the electron-phonon attraction $V<0$ in the Debye-layer determined by $\hbar\omega_D=0.06$ eV [13]. The repulsive interband coupling is characterized by the constant $W>0$. Interactions U and W are operative in the energy interval from E_c to zero (σ-band top). The cut-off energy E_c determines the bands overlap region and is taken as $E_c=-2$ eV. Then the chemical potential of the undoped MgB_2 is $\mu=-0.6$ eV [7]. We characterize the effective σ- and π-bands by constant densities of states $\rho_1=0.25$ and $\rho_2=0.11$ (eV^{-1}) [7].

The necessary values of the interaction constants have been determined in [12] by simultaneous fitting of experimental data for T_c, the specific heat jump and the ratio of zero-temperature gaps. As a result $V_1=$

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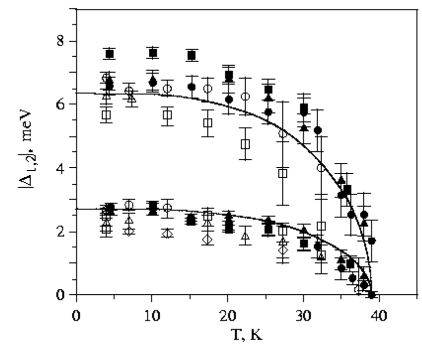

Fig. 1. The MgB_2 superconductivity gaps *vs* temperature. Solid line - theory. Filled symbols - the experimental data of [2]; open symbols - the experimental data of [14].

-1.01 and $W = 0.53$ (eV) have been chosen, and according to an estimation $U = 1$ eV [12].

The temperature dependencies of the gaps on the Fermi level calculated from (2) agree well with the measured ones [2,14], as it is seen from Fig. 1.

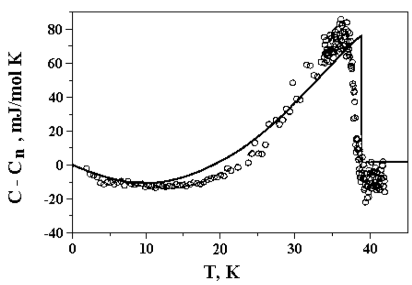

Fig. 2. The MgB_2 specific heat *vs* temperature. Solid line - theory. Points represent the experimental data of [15].

On the basis of Eqs. (1),(2) one can find the thermodynamic characteristics for MgB_2. Theoretical curve of specific heat *vs* temperature in Fig.2 follows the experimental data of [15]. In Fig.3 the calculated temperature dependence of H_{C2} describes satisfactory the experimental data of [16]. At this the Ginzburg-Landau parameter value κ=38 [4] has been used.

For the calculation of $T_c(x)$ for $Mg_{1-x}Al_xB_2$ we have taken account of $\rho_{1,2}$ changes in the Debye layer near E_F with doping according to[8]. The result is shown in Fig.4 together with the experimental points from [17].

In conclusion, the model of present type seems to be able to describe the properties of the two-gap superconductor MgB_2.

Acknowledgements

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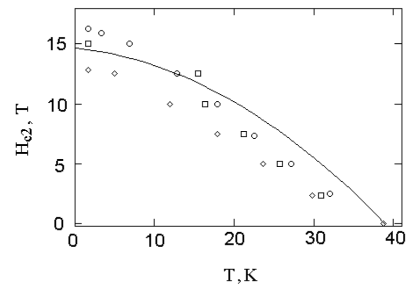

Fig. 3. The MgB_2 critical magnetic field H_{C2} *vs* temperature. Solid line - theory. Points represent the experimental data of [16].

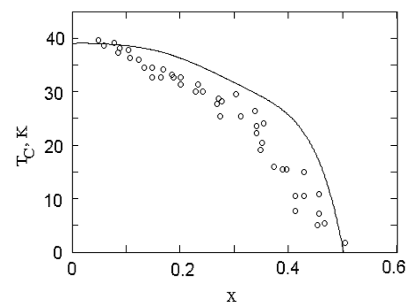

Fig. 4. The influence of doping on T_c in $Mg_{1-x}Al_xB_2$. Solid line - theory. Points represent the experimental data of [17].

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