TT 18.2 Mo 10:30 TU H2053

Interband Pairing Interaction in the Two-Band Superconductor MgB_2 Observed by Tunneling — •J. Geerk[1], R. Schneider[1], G. Linker[1], A. Zaitsev[1], R. Heid[1], K.-P. Bohnen[1], and H. v. Löhneysen[1,2] — [1]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, P.O.B. 3640, D-76021 Karlsruhe — [2]Physikalisches Institut, Universität Karlsruhe

The anisotropic superconductor MgB_2 was studied by tunneling spectroscopy of tunnel junctions of the sandwich type prepared on as deposited thin films with T_c values near 32 K. The tunnel junctions revealed an energy gap between 2.5 and 3 meV and phonon induced structures in the tunnelling density of states. The inversion of the tunnel data using the standard single-band Eliashberg equations yielded a so-called effective Eliashberg function with three distinct peaks at 38,58 and 85 meV which is compared to a theoretical calculated counterpart obtained by inversion of superconducting density of states data from two-band Eliashberg equations where electron-phonon spectral functions extracted from ab-initio LDA calculations were inserted. Convincing agreement is found between the experimental and calculated effective Eliashberg functions. Further evaluation reveals that the central peak a 58 meV mainly reflects the shape of the π-σ interband pairing interaction which appears in the gap function of the π-sheet in an amplified way due to the large gap of the σ-sheet. It is concluded that the superconductivity on the π-sheet is essentially generated by interband electron-phonon coupling.

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Mixing between ballistic and diffusive motion in superconducting MgB_2 — •Matthias Eschrig[1], Kaori Tanaka[2,3], Daniel Agterberg[4], and Juha Kopu[5] — [1]Institut für Theoretische Festkörperphysik, Universität Karlsruhe, 76128 Karlsruhe, Germany — [2]Department of Physics and Engineering Physics, University of Saskatchewan, Saskatoon, SK, Canada S7N 5E2 — [3]Argonne National Laboratory, Argonne, IL 60439, U.S.A. — [4]Department of Physics, University of Wisconsin-Milwaukee, P.O. Box 413, Milwaukee, WI 53211, U.S.A — [5]Low Temperature Laboratory, Helsinki University of Technology, PO Box 2200, FIN-02015 HUT

We introduce a model for the two-band superconductor MgB_2 in which the motion of quasiparticles is diffuse in one band (the π-band) and ballistic in the other band (the σ-band). Diffusive and ballistic quasiparticles are coupled by the pairing interaction. We apply this model to examine the electronic structure of vortex cores in MgB_2. In particular, we study the effects of impurities on the ballistic motion of quasiparticles in the σ-band in the vortex core region under the presence of the hybridization with the diffusive π-band.We find that the induced superconductivity in the π band results in a core size larger than estimated by H_{C2} and in weakly bound states, and that those bound states are removed easily by impurities.

TT 18.4 Mo 11:00 TU H2053

Band filling and interband scattering effects in MgB_2: C vs Al doping — •Jens Kortus[1], O.V. Dolgov[2], R.K. Kremer[2], and A.A. Golubov[3] — [1]Institut de Physique et Chimie des Matériaux de Strasbourg, 23 rue du Loess, F-67034 Strasbourg Cedex 2, France — [2]MPI-FKF, Heisenbergstr. 1, 70569 Stuttgart — [3]MESA+ Research Institute and Faculty of Science and Technology, University of Twente, 7500 AE Enschede, The Netherlands

We argue, based on band structure calculations and Eliashberg theory, that the observed decrease of T_c of Al and C doped MgB_2 samples can be understood mainly in terms of a band filling effect due to the electron doping by Al and C. A simple scaling of the electron-phonon coupling constant λ by the variation of the density of states as function of electron doping is sufficient to capture the experimentally observed behavior. Further, we also explain the long standing open question of the experimental observation of a nearly constant π gap as function of doping by a compensation of the effect of band filling and interband scattering. Both effects together generate a nearly constant π gap and shift the merging point of both gaps to higher doping concentrations, resolving the discrepancy between experiment and theoretical predictions based on interband scattering only.

TT 18.5 Mo 11:15 TU H2053

Density functional theory for superconductors: Applications to MgB_2 and solids under pressure — •Andrea Floris[1], Cesare Franchini[2], Nektarios Lathiotakis[1], Gianni Profeta[3], Sandro Massidda[2], and E. K. U. Gross[1] — [1]Institut für Theoretische Physik, Freie Universität Berlin, Germany — [2]INFM SLACS, Sardinian Laboratory for Computational Materials Science and Dipartimento di Scienze Fisiche, Università degli Studi di Cagliari, Italy — [3]C. A. S. T. I. - Istituto Nazionale Fisica della Materia (INFM) and Dipartimento di Fisica, Università degli studi dell' Aquila, Italy

Understanding and predicting the properties of superconductors is of both fundamental and technological importance. The discovery of superconductivity in MgB_2, of its rather high critical temperature (T_c = 39.5K), and the appearance of multiple gaps, has renewed the interest in conventional superconductivity. Here we present several applications of a novel approach to superconductivity that allows one to calculate material-specific properties, such as the gap and the T_c, in a truly ab-initio fashion without using any adjustable parameters. Within this approach, we obtained the T_c and the two gaps of MgB_2 in good agreement with experiment, taking into account the strong anisotropy of both the electron-phonon and the Coulomb interactions. As a further application, we studied the behaviour of T_c in Li and Al as a function of pressure. Despite their common simple metal structure, these materials show different behaviour upon pressure. While Li undergoes several transitions favouring superconductivity, in Al the electron-phonon coupling decreases with pressure leading to a complete suppression of Tc around 8GPa.

TT 18.6 Mo 11:30 TU H2053

Multi-band influence on superconductivity in $HoNi_2B_2C$ — •A. Wälte[1], G. Fuchs[1], Yu.G. Naidyuk[2], K. Nenkov[1], S.-L. Drechsler[1], D. Souptel[1], H. Rosner[3], J. Freudenberger[1], K.-H. Müller[1], G. Behr[1], and L. Schultz[1] — [1]Institut für Festkörper- und Werkstoffforschung Dresden, Helmholtzstr. 20, D-01171 Dresden — [2]B. Verkin Institute for Low Temperature Physics and Engineering, National Academy of Sciences of Ukraine, 47 Lenin Ave., 61103 Kharkiv, Ukraine — [3]MPI CPFS Dresden, Nöthnitzer Str. 40, D-01187 Dresden

Rare-earth nickel borocarbides RNi_2B_2C reveal, depending on the rare-earth R, superconductivity, magnetism or even a mixture of these competing phenomena [1]. The reduction of the superconducting ordering temperature T_c by magnetic pair-breaking fairly follows the Abrikosov-Gorkov model. However, details of the influence of magnetism on the electron system are not yet well understood. From specific heat measurements and point-contact spectroscopy on $HoNi_2B_2C$ the phonon density of states $F(\omega)$ and the spectral function $\alpha^2F(\omega)$ have been extracted. The characteristic phonon frequency $\omega_{\ln} \approx 180$ K is similar to $\omega_{\ln}$ of non-magnetic $LuNi_2B_2C$. Comparing the specific heat jumps of both compounds, an unexpectedly strong deviation from the Abrikosov-Gorkov expectation for $HoNi_2B_2C$ is found. A possible explanation is the different influence of pair-breaking on different electron bands.

[1] R.J. Cava et al., Nature 367, January 1994.

TT 18.7 Mo 11:45 TU H2053

Are intercalated metallochloronitrides electron-phonon mediated superconductors? — •Rolf Heid and Klaus-Peter Bohnen — Institut für Festkörperphysik, Forschungszentrum Karlsruhe

The layered metallochloronitrides XNCl, X=Zr,Hf, have surprised with rather high superconducting transition temperatures of up to 25.5 K after intercalation with Li or Na [1], raising the question to what extent the conventional electron-phonon coupling mechanism is at work. Here we present results of an ab initio investigation of the lattice dynamics and electron-phonon coupling of undoped and Li-intercalated ZrNCl applying a density-functional perturbation approach, which allows a calculation of the full momentum dependency of these quantities. The theoretical phonon spectra are found to be in very good agreement with those obtained by neutron scattering experiments [2]. On intercalation, small Fermi surface pockets develop around the K points. This topology gives rise to strongly momentum dependent electron-phonon coupling, which is carried predominantly by two in-plane vibrations of Zr and N. We find that the integrated coupling constant is ≈ 0.5, a value significantly larger than estimated before [3], but still rather small in view of the high T_c values observed. Implications for the superconducting mechanism will be discussed.

[1] S. Yamanaka *et al.*, Nature **392**, 580 (1998)
[2] P.Adelmann *et al.*, J. Low Temp. Phys. **117**, 449 (1999)
[3] R. Weht *et al.*, Europhys. Lett. **48**, 320 (1999)