TT 18 Superconductivity: Borides, Borocarbides, Carbides, ...

Time: Tuesday 15:00–18:30 Room: HSZ 02

TT 18.1 Tue 15:00 HSZ 02

Three-Dimensional MgB_2-Type Superconductivity in Hole-Doped Diamond — •Jens Kortus[1], Lilia Boeri[2], and Ole K. Andersen[2] — [1]Theoretische Physik, TU Bergakademie Freiberg, Germany — [2]MPI FKF Stuttgart, Germany

We substantiate by numerical and analytical calculations that the recently discovered superconductivity in boron-doped diamond is caused by electron-phonon coupling of the same type as in MgB_2, albeit in three dimensions. Using first-principles linear response methods based on density functional theory we obtain the phonon dispersion and the electron-phonon coupling strength as function of hole doping. As revealed by these calculations, holes at the top of the zone-centered, degenerate sigma-bonding valence-band couple strongly to the optical bond-stretching phonon modes. This mechanism shows several very similar aspects to the one which drives the superconductivity in MgB_2. However, the increase from two dimensions in MgB_2 to three dimensions in diamond reduces the phonon mode softening crucial for the high T_c of 40 K in MgB_2. Even if diamond had the same bare coupling constant as MgB_2, which could be achieved with higher doping, Tc would be limited to only 25 K. Using the same theoretical methods we also investigate the possibility of superconductivity in the isostructural and isoelectronic semiconductors Si and Ge. Superconductivity above 1 K in Si (Ge) requires hole doping beyond 5% (10%).

L. Boeri, J. Kortus, O.K. Andersen, Phys. Rev. Lett. 93, 237002 (2004)

TT 18.2 Tue 15:15 HSZ 02

Superconductivity and electron phonon coupling in doped MgB_2 compounds — •Vivien Petzold[1] and Helge Rosner[2] — [1]TU Dresden — [2]MPI for Chemical Physics of Solids Dresden

Recently, substitutions on the metallic site in MgB_2, e.g. $Mg_{1-x}Sc_xB_2$ [1], $Mg_{1-x}(AlLi)_xB_2$ [2] and $Nb_{1-x}B_2$ [3] were investigated intensively. For the achievable doping levels (x=0.12...0.27) in $Mg_{1-x}Sc_xB_2$, the compound shows only very small structural changes, allowing the separation of lattice and doping effects. On the other hand $Mg_{1-x}(AlLi)_xB_2$ is isoelectronical to MgB_2, but varies in lattice constants depending on x. In order to investigate the influence of the degree of substitution on the electronic properties, we present band structure calculations using different levels of approximation: rigid band and virtual crystal approach as well as supercell calculations and coherent potential approximation. We show that the latter two approaches lead to consistent results with respect to lattice expansion and electronic properties (density of states, Fermi surfaces). We demonstrate that in the transition metal (T) diborides the doping dependent changes in the electronic structure are strongly influenced by the sp^2(B)-d(T) hybridization. The influence of the doping on the electron phonon coupling is discussed.

[1] Agrestini et al. Phys. Rev. B **70** 134514 (2004).
[2] Monni et al. cond-mat 0506162 (2005).
[3] Yamamoto et al. Physica C 383 (2002) 197-206.

TT 18.3 Tue 15:30 HSZ 02

Density functional theory for superconductors: Applications to MgB_2 and Pb — •A. Floris[1], N. Lathiotakis[1], A. Sanna[2], C. Franchini[2], M. Marques[3], M. Lueders[4], G. Profeta[5], A. Continenza[5], S. Massidda[2], and E.K.U. Gross[1] — [1]Freie Universitaet Berlin, Arnimallee 14, D-14195 Berlin, Germany — [2]INFM SLACS and Dipartimento di Scienze Fisiche, Universita' degli Studi di Cagliari, Italy — [3]Institut de Minéralogie et de Physique des Milieux Condensés, Université Pierre et Marie Curie - Paris VI, France — [4]Daresbury Laboratory, Warrington WA4 4AD, United Kingdom — [5]C.A.S.T.I. - INFM and Dipartimento di Fisica, Universita' degli studi dell'Aquila, Italy

Predicting the properties of superconductors is of both fundamental and technological importance. The discovery of superconductivity in MgB_2 (T_c=39.5 K), with a clear presence of two gaps, has renewed the interest in conventional superconductivity. Here we present two applications of a novel approach to superconductivity that allows one to calculate material-specific properties without using any adjustable parameters. Within this approach, we have obtained the critical temperature 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. Moreover, in a fully k-resolved formalism, we find two different gaps also in Pb, and we relate this fact to the difference in strength of the electron-phonon coupling associated with the two bands crossing the Fermi level. This calculation shows how our formalism is able to capture, in absence of any ad-hoc model, the features of multi-gap superconductors.

TT 18.4 Tue 15:45 HSZ 02

Specific heat of $Mg(B_{1-x}C_x)_2$: Two Superconducting Gaps — •Niels Oeschler[1,2], Robert A. Fisher[1], Norman E. Phillips[1], William E. Mickelson[1], and Alex Zettl[1] — [1]University of California, Berkeley, CA, USA — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

We present specific heat data of polycrystalline $Mg(B_{1-x}C_x)_2$ with $x = 0.1$ and 0.2 from 1K to 35K in magnetic fields up to 9T.
Recently, MgB_2 was identified as a phonon-mediated two-gap superconductor with remarkably high transition temperature of 39K. The small gap and the large gap open at the same temperature due to interband coupling. Substituting carbon on the boron site has the effect of electron filling and inducing disorder. The superconducting transition temperature decreases monotonically from 39K for MgB_2 to 20K for $Mg(B_{0.8}C_{0.2})_2$. The specific heat of both samples can be accurately fitted with two superconducting energy gaps using the extended α model. The amplitudes of the gaps are found to be larger than the BCS value for the large gap and smaller than the BCS value for the small gap. However, it is observed that the size of both gaps decreases upon increasing the carbon content.
The evolution of the gap sizes, the normal-state Sommerfeld coefficients, the Debye temperatures and the critical fields are compared to those of MgB_2.

TT 18.5 Tue 16:00 HSZ 02

Superconducting properties of the 13 K rare earth carbide superconductor, La_2C_3 — •Jun Sung Kim, Reinhard K. Kremer, Volodymyr Babizhetskyy, Ove Jepsen, and Arndt Simon — MPI-FKF, 70569 Stuttgart

Superconductivity in rare earth carbides has attracted interest again after the recent discovery of the 18 K superconductor Y_2C_3.[1] We have successfully synthesized the related La system, La_2C_3, and after a careful control of the carbon content and the annealing procedures, optimized the superconducting properties reaching at sharp transition temperature $T_c \sim 13.2$ K. The superconducting properties have been investigated by heat capacity measurements in magnetic fields up to H= 9 T, resistivity and magnetization measurements up to H = 30 T. The characteristic specific heat anomaly is compared to the predictions of the BCS and the α model, and a quantitative estimate of the electron-phonon coupling strength and the logarithmic average phonon frequency is made. From a detailed analysis including full potential electronic structure calculations based on the refined structure gained from the refinement of low-temperature neutron powder diffraction experiments, La_2C_3 is found to be in the strong electron-phonon coupling regime. The upper critical fields show a clear enhancement with respect to the Werthamer-Helfand-Hohenberg prediction and amount to $\sim$ 20 T at 0 K.

[1] G. Amano, S. Akutagawa, T. Muranaka, Y. Zenitani, and J. Akimutsu, J. Phys. Soc. Jpn. **73**, 530 (2004).

— 15 min. break —

TT 18.6 Tue 16:30 HSZ 02

Soft-mode behavior in superconducting MgB_2-like ternary silicides MAlSi (M=Ca,Sr,Ba) — •R. Heid[1], K.-P. Bohnen[1], B. Renker[1], P. Adelmann[1], D. Ernst[1], and H. Schober[2] — [1]Forschungszentrum Karlsruhe, Institut für Festkörperphysik — [2]Institut Laue-Langevin, Grenoble

The discovery of superconductivity with $T_c \approx$ 39K in MgB_2 has led to an intensive search for new superconductors with similar layered structures. Among them, the ternary silicides MAlSi with M=Ca,Sr,Ba exhibit interesting electronic and superconducting properties. With increasing mass of the M ion, T_c drops from 7.8K (Ca) to 5.1K (Sr) to <2K (Ba). Electronic structure calculations suggest that all three compounds possess very similar electronic properties [1], thus pointing to significant differences in the phonons and electron-phonon coupling (EPC).

Here we present results of a combined experimental and theoretical investigation of the lattice dynamics and EPC of the series MAlSi, M=Ca,Sr,Ba. Inelastic neutron-scattering measurements of the generalized phonon density of states show evidence for a low-frequency phonon mode in CaAlSi, which stiffens with increasing mass of the M ion. Using density-functional perturbation calculations of the phonons and EPC, we could identify this mode as an out-of-plane Al vibration with a large EPC. Contrary to a previous theoretical study [2], we do not find evidence for a dynamical instability. We will discuss implications for the observed superconducting trends among the MAlSi series.

[1] I. I. Mazin *et al.*, Phys. Rev. B**69**, 180512 (2004)
[2] G. Q. Huang *et al.*, Phys. Rev. B**69**, 064509 (2004)

TT 18.7 Tue 16:45 HSZ 02

Lattice dynamics and electron-phonon interaction in doped small radius nanotubes — •K.-P. Bohnen[1], R. Heid[1], H.J. Liu[2,3], and C.T. Chan[2] — [1]Forschungszentrum Karlsruhe, Institut für Festkörperphysik — [2]Dept. of Phys., Univ. of Sci. and Technology, Kowloon, HongKong — [3]Dept. of Phys., Wuhan Univ., Wuhan, People's Republic of China

Recently lattice dynamics of small radius nanotubes has received a lot of attention due to the competition between superconductivity and Peierls transition. So far all ab-initio calculations for isolated nanotubes with diameter of 4 Å have shown a strong tendency to either a Peierls transition (in (3,3)-tubes)[1] or a structural transition to a non-metallic state with a small gap ((5,0)-tube) [2], in contrast to experimental findings of superconductivity in 4 Å tubes [3]. Doping these tubes might offer a possibility to enhance superconductivity, an effect which is well known from intercalated graphite. We present here ab-initio calculations of the lattice dynamics and electron-phonon coupling for doped (3,3)-tubes. The doping level has been chosen to move the Fermi level to a region of high density of states, however so far these calculations still favor the Peierls transition compared to superconductivity.

[1] K.-P. Bohnen, R. Heid, H.J. Liu, C.T. Chan, PRL **93**, 245501 (2004)
[2] D. Connetable et al., PRL **94**, 015503 (2005)
[3] Z.K. Tang et al., Science **292**, 2462 (2001)

TT 18.8 Tue 17:00 HSZ 02

Strong electron-phonon coupling in YNi_2B_2C: Theory and Experiment — •F. Weber[1,2], A. Kreyssig[3], L. Pintschovius[1], K. Hradil[4], K.-P. Bohnen[1], R. Heid[1], and W. Reichardt[1] — [1]Forschungszentrum Karlsruhe, Inst. f. Festkörperphysik — [2]Fak. f. Physik, Univ. Karlsruhe — [3]IAPD, TU Dresden — [4]PCI, Univ. Göttingen

Several compounds of the family $RENi_2B_2C$ (RE=Y, Lanthanoid) exhibit high superconducting transition temperatures (up to about 20 K) which is thought to be due to strong electron-phonon coupling (EPC). We made extensive calculations using density functional theory which indeed predict an EPC strength sufficient to explain the observed T_c's. We note that the strong EPC gives rise to pronounced anomalies in the phonon dispersion curves and concurrently to large line widths of certain phonon modes. In particular, there should be a pronounced phonon anomaly at the zone boundary in the (110)-direction (the so-called M-point) in addition to the already known anomaly in the (100)-direction. Inelastic neutron scattering measurements were performed on YNi_2B_2C on the triple axis spectrometer PUMA, Munich. The data show an extremely good agreement between the predicted and the observed phonon frequencies. Moreover, the measurements confirm the strong line broadening of the anomalous M-point mode predicted by theory. Finally, measurements in different Brillouin zones confirm the theoretical predictions, that in spite of the low frequency of the anomalous mode its eigenvector contains rather large amplitudes of the light atoms B and C.

TT 18.9 Tue 17:15 HSZ 02

Single crystal X-ray diffraction analysis and electron density calculation of YNi_2B_2C — •T. Leisegang[1], D. C. Meyer[1], P. Paufler[1], D. Souptel[2], G. Behr[2], O. Ignatchik[3], A. Ormeci[4], H. Rosner[4], and J. Wosnitza[5] — [1]ISP, TU Dresden, Germany — [2]IFW-Dresden, Germany — [3]IFP, TU Dresden, Germany — [4]MPI-CPfS, Germany — [5]HLD Dresden, FZ Rossendorf, Germany

The quaternary borocarbide YNi_2B_2C, space group (139) $I4/mmm$, exhibits superconductivity ($T_c \approx 15$ K) as was first reported in [1]. This superconducting behaviour depends strongly on the crystal composition within the small homogeneity range and on the crystal growth conditions. Here we report on investigations of two different samples, namely bulk samples grown by a floating zone technique [2] and plate samples grown by a flux-growth method [3]. De Haas-van Alphen (dHvA) measurements were performed to determine the electronic band structure as well as the evolution of a superconducting energy gap at the Fermi surface [4]. To evaluate the exact crystal structure, single-crystal X-ray diffraction measurements at room temperature were performed. Different models of structural disorder were refined and a difference-Fourier analysis was carried out. The experimental electron density will be compared with theoretical calculations. The work was supported by the Deutsche Forschungsgemeinschaft (SFB 463).

[1] Nagarajan et al., Phys. Rev. Lett. 72, 274 (1994).
[2] Souptel et al., J. Cryst. Growth 276, 652 (2005).
[3] Canfield et al., Phys. Today 51, 40 (1998).
[4] Ignatchik et al., J. Magn. Magn. Mat. 290-291, 424 (2005).

TT 18.10 Tue 17:30 HSZ 02

The Fermi surface topology and the superconducting gap function in UPd_2Al_3: a neutron spin-echo study — •Arno Hiess[1], Elizabeth Blackburn[1,2], Maikel C. Rheinstädter[1], Wolfgang Häussler[1,3], Nicholas Bernhoeft[4], and Gerry H. Lander[2] — [1]Institut Laue-Langevin, BP 156, F-38042 Grenoble, France — [2]European Commission, JRC, ITU, Postfach 2340, D-76125 Karlsruhe, Germany — [3]FRM-II, TU München, D-85748 Garching, Germany — [4]DRFMC, CEA-Grenoble, F-38054 Grenoble, France

We report on a single crystal neutron spin-echo investigation of the low-energy dynamic response in the magnetic superconductor UPd_2Al_3 ($T_N = 14$ K, $T_{sc} = 2$ K) in the vicinity of the antiferromagnetic wavevector $Q_0 = (0\ 0\ 0.5)$. Well inside the superconducting phase, antiferromagnetic quasielastic scattering, which is present in the normal state, is absent for relaxation times shorter than 10 ns, equivalent to an energy resolution better than 1 μeV. These observations are related to the geometry of the gap function and the Fermi surface topology. Any nodes present at the Fermi surface do not contribute significant weight to the electronic susceptibility. This places strong constraints on possible models for the origin and role of magnetic excitations in this magnetic superconductor.

TT 18.11 Tue 17:45 HSZ 02

Superconductivity and Lattice Instability in Compressed Lithium from Fermi Surface Hot Spots — •Deepa Kasinathan[1], Jan Kunes[1], Amy Lazicki[1,2], Helge Rosner[3], Choong-shik Yoo[2], Richard Scalettar[1], and Warren Pickett[1] — [1]Dept. of Physics, University of California - Davis, CA 95616, U.S.A — [2]Lawrence Livermore National Labratory, Livermore, CA — [3]Max-Planck-Institute for Chemical Physics of Solids, Dresden, Germany

Lithium, a simple metal not su perconducting above 5mK at ambient pressure, becomes a 20 K superconductor at 50 GPa. This high T_c is shown to arise from critical (formally divergent) electron-phonon coupling to the transverse phonon branch along intersections of Kohn anomaly surfaces with the Fermi surface. First principles linear response calculations of the phonon spectrum and spectral function $\alpha^2F(\omega)$ reveal (harmonic) instability already at 25 GPa. Our results imply that the fcc phase is anharmonically stabilized in the 25-38 GPa range.

TT 18.12 Tue 18:00 HSZ 02

Cooper pairing on a sphere: multielectron bubbles in helium — •Jacques Tempere[1,2], Vladimir Gladilin[1], Jozef Devreese[1], and Isaac Silvera[2] — [1]TFVS, Universiteit Antwerpen, Universiteitsplein 1, 2610 Antwerpen, Belgium — [2]Lyman Laboratory of Physics, Harvard University, Cambridge MA, USA

Electrons on helium constitute a versatile realization of a two-dimensional electron gas. Multielectron bubbles are cavities inside liquid helium, containing electrons that collect at the surface of the bubble, forming a spherical two-dimensional electron gas. In this contribution, we investigate the effects of the electron-ripplon interaction on the spherical electron system. We derive the conditions for which the electron-ripplon interaction can lead to an attractive interaction between the electrons, and to pairing. The paired state is described using Richardson's method. The density of states, the pair-breaking gap, and the ground state level occupations are derived and discussed. The difference between Cooper pairing in a flat electron system and Cooper pairing on a sphere are highlighted. Finally, progress in the experimental realization of this system is discussed.