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 $\mu$eV. 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.