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Non-centrosymmetric CePt₃Si and CePt₃B and their mechanical properties

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The first non-centrosymmetric heavy fermion superconductor CePt₃Si [1], crystallizing with CePt₃B -type, without an inversion symmetry (one of the key symmetries for Cooper pairing) shows a number of novel physical properties. In order to get insight into the pressure dependence of the strong electron correlations in these materials the present paper provides mechanical property data (elastic moduli and hardness both at room temperature as well as thermal expansion in the range from 4.2 to 670 K) for both single and polycrystalline CePt₃Si and its prototype compound CePt₃B.

The experimental data are backed by first-principles (ab-initio) calculation. Resonant ultrasound spectroscopy was used to determine elastic properties (Young's elastic modulus E and Poissons ratio ν) via the eigenfrequencies of the sample and the knowledge of sample mass and dimensions. Bulk modulus and shear modulus were calculated from E and ν , and with Anderson's equation the respective Debye temperatures were derived. In addition, ab-initio DFT calculations were carried out for both compounds. A comparison with parameters evaluated from these first-principles computations with the experiments revealed, in general, good agreement. Positive and negative thermal expansion values obtained from CePt₃Si single crystal data are fairly well explained in terms of the crystalline electric field model, using CEF parameters derived recently from inelastic neutron scattering. The DFT calculations, in addition, demonstrate that the atomic vibrations keep almost unaffected by the antisymmetric spin-orbit coupling present in systems with crystal structures having no inversion symmetry. This is opposite to electronic properties, where the antisymmetric spin-orbit interaction has shown to distinctly influence features like the superconducting condensate of CePt₃Si.

[1] E. Bauer, G. Hilscher, H. Michor, C. Paul, E.W. Scheidt, A. Grybanov, Yu. Seropegin, H. Noel, M. Sigrist and P. Rogl; "Heavy Fermion Superconductivity and Magnetic Order in Non-centrosymmetric CePt₃Si", *Phy. Rev. Lett.*, 92, 027003 (2004)1-4.

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