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Impact of lattice dynamics on the phase stability of metamagnetic FeRh: Bulk and thin films MICHAEL WOLLOCH, Vienna University of Technology, MARKUS E. GRUNER, WERNER KEUNE, University of Duisburg-Essen, PETER MOHN, JOSEF REDINGER, FLORIAN HOFER, DIETER SUESS, Vienna University of Technology, RAIMUND PODLOUCKY, University of Vienna, JOACHIM LANDERS, SOMA SALAMON, FRANZISKA SCHEIBEL, DETLEF SPODDIG, University of Duisburg-Essen, RALF WITTE, Karlsruhe Institute of Technology, BEATRIZE ROLDAN CUENYA, Ruhr-University Bochum, OLIVER GUTFLEISCH, TU Darmstadt, MICHAEL Y. HU, JIYONG ZHAO, THOMAS TOELLNER, ERCAN E. ALP, Argonne National Laboratory, MARIO SIEWERT, PETER ENTEL, ROSSITZA PENTCHEVA, HEIKO WENDE, University of Duisburg-Essen — We present phonon dispersions, element-resolved vibrational density of states (VDOS) and corresponding thermodynamic properties obtained by a combination of density functional theory (DFT) and nuclear resonant inelastic x-ray scattering (NRIXS) across the metamagnetic transition of B2 FeRh in the bulk material and thin epitaxial films. We see distinct differences in the VDOS of the antiferromagnetic (AF) and ferromagnetic (FM) phases, which provide a microscopic proof of strong spin-phonon coupling in FeRh. In the bulk phase, lattice vibrations contribute with the same sign and in similar magnitude to the isostructural AF-FM phase transition as excitations of the electronic and magnetic subsystems demonstrating that lattice degrees of freedom need to be included in thermodynamic modeling. We also propose a new monoclinic groundstate.

Michael Wolloch
Vienna University of Technology

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