Supplementary Materials: Calculation of T_c of superconducting elements with the Roeser-Huber formalism

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The Supplementary Materials include the drawings of the superconducting paths for each crystal structure (rhombohedral, tetragonal bcc, hcp, fcc* and dhcp) investigated in the paper. The numbering of the paths corresponds to Tables I and II in the paper.

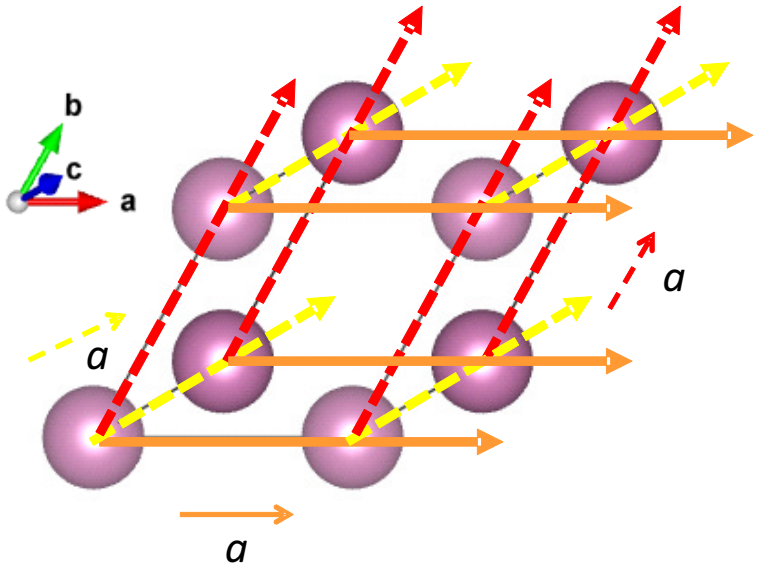


Figure S1. The rhombohedral crystal structure of α-Hg. The details of this crystal structure were already discussed by Roeser et al. [1]. All 3 directions are equal, and the only relevant interatomic distance is given by a. Each path belongs to two unit cells, so only one superconducting path must be considered in the calculation of T_c.

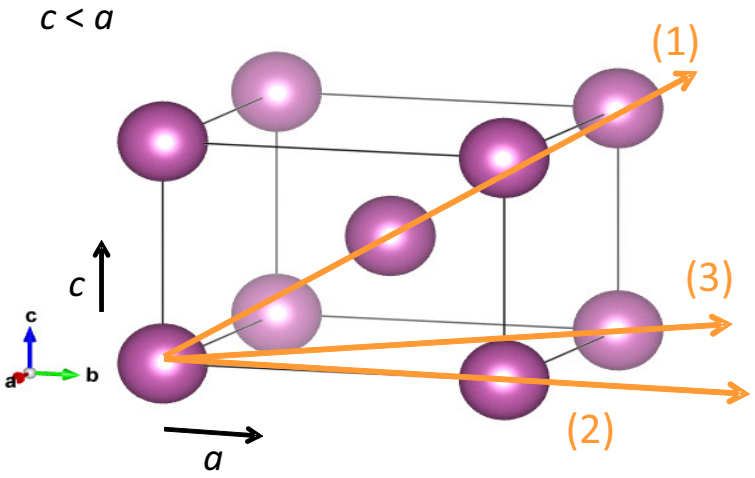


Figure S2. The tetragonal bcc structure of β-Hg. The possible superconducting paths are the same as in the regular bcc structure, except that $c < a$. The paths fulfilling the symmetry condition are given by the orange vectors (1) – (3).

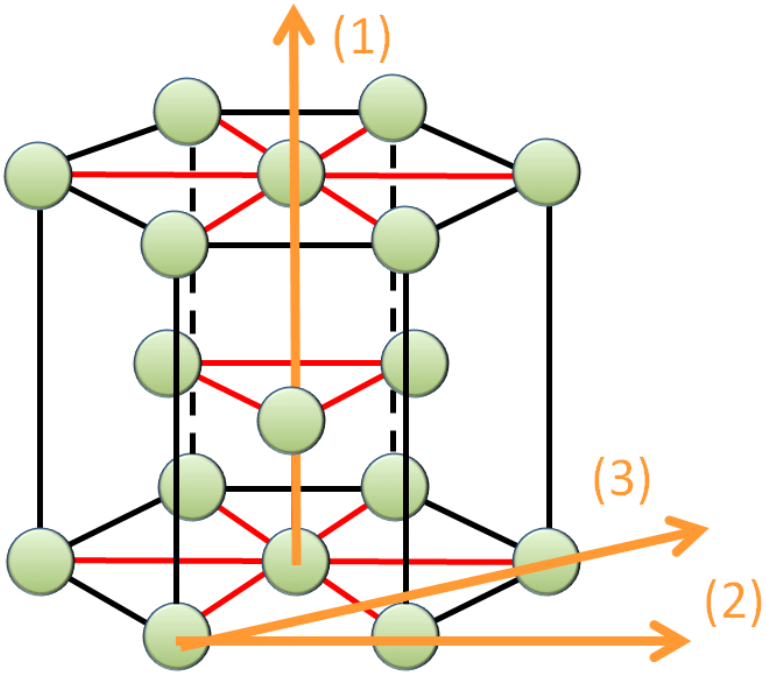


Figure S3. The hcp crystal structure, which is the base for the other two structures, fcc* and dhcp. The superconducting paths fulfilling the symmetry condition are given by the orange vectors (1) – (3).

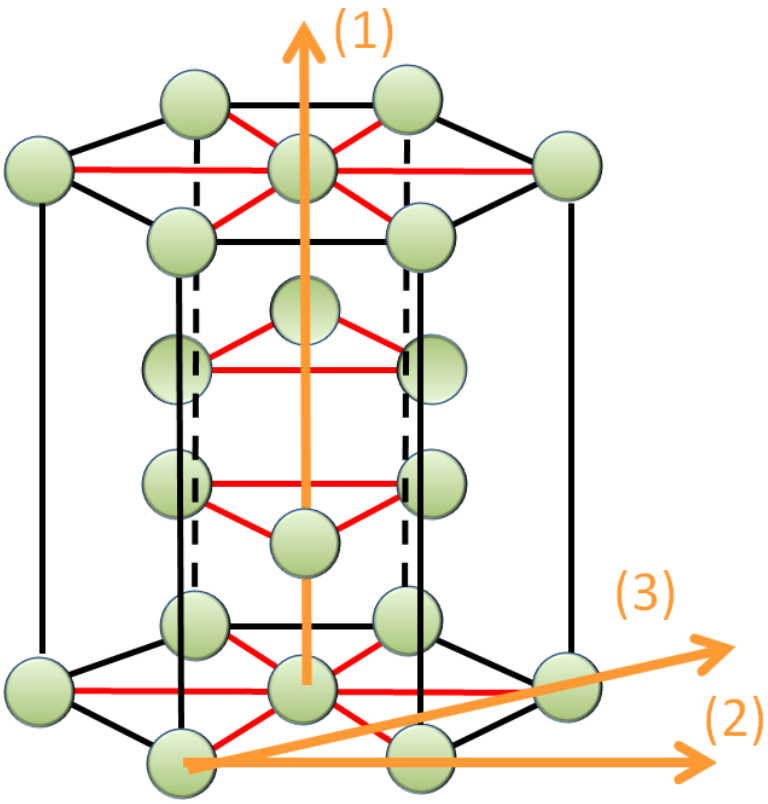


Figure S4. The fcc* crystal structure in [111]-direction (found for La, Ce and Yb [2]), showing one additional inner layer as compared to the hcp structure. The superconducting paths fulfilling the symmetry condition are given by the orange vectors (1) – (3).

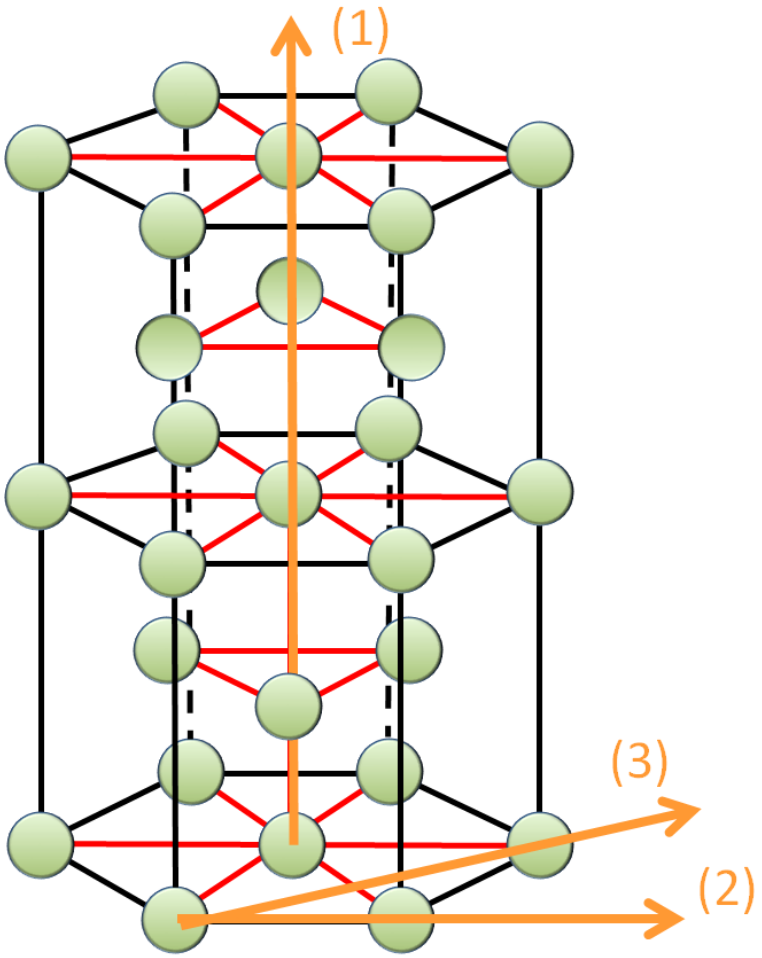


Figure S5. The dhcp crystal structure which is unique to the rare earth materials. The superconducting paths (1) – (3) are the same as for the fcc*-structure, but one must note the different length for *c* due to the central atom in the middle plane.

References

1. Roeser, H.P.; Haslam, D.T.; Lopez, J.S.; Stepper, M.; von Schoenermark, M.F.; Huber, F.M.; Nikoghosyan, A.S. Correlation between transition temperature and crystal structure of niobium, vanadium, tantalum and mercury superconductors. *Acta Astronaut.* **2010**, *67*, 1333–1336, doi:10.1016/j.actaastro.2010.06.048.
2. Gschneidner, K. A., Jr.; Pecharsky, V. K. Rare-earth elements. *Encyclopedia Britannica*, 17 Jan. 2019, https://www.britannica.com/science/rare-earth-element/Properties-of-the-metals#/media/1/491579/173111 (accessed on 31. 01. 2022).