Supplementary Materials for

"Superconductivity above 30 K Achieved in Dense Scandium"

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I. Experiments

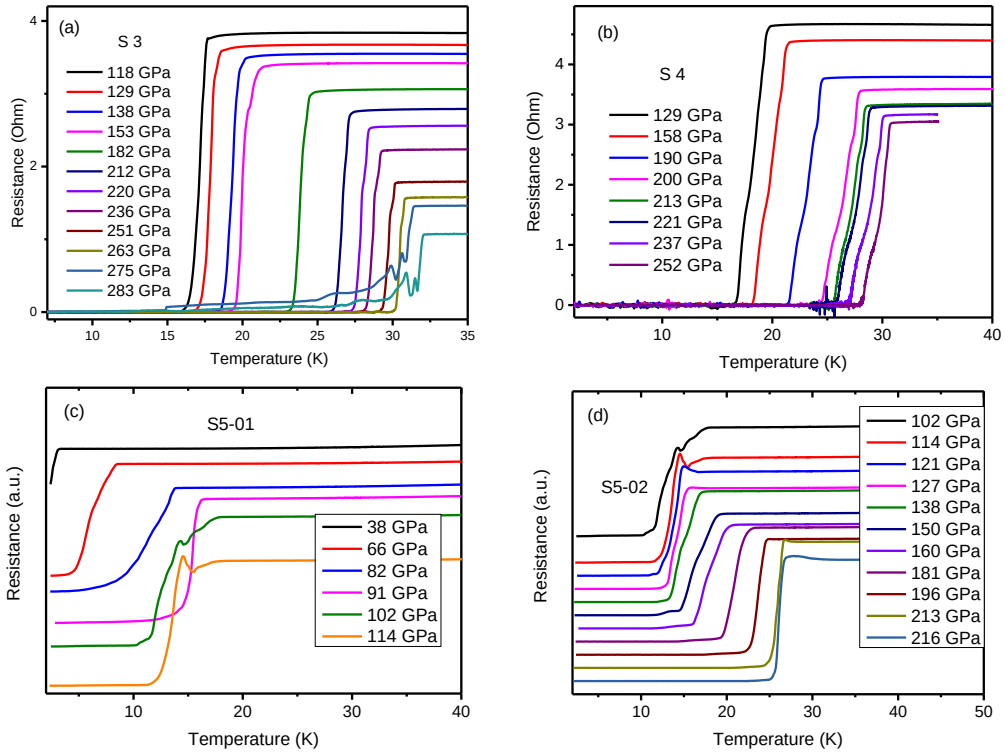

Fig. S1 (a~d) Temperature dependence of the electrical resistance of elemental Sc metal measured at high pressures for sample 3~5. Sample 3 and 4 are Sc thin foils while sample 5 are Sc powder.

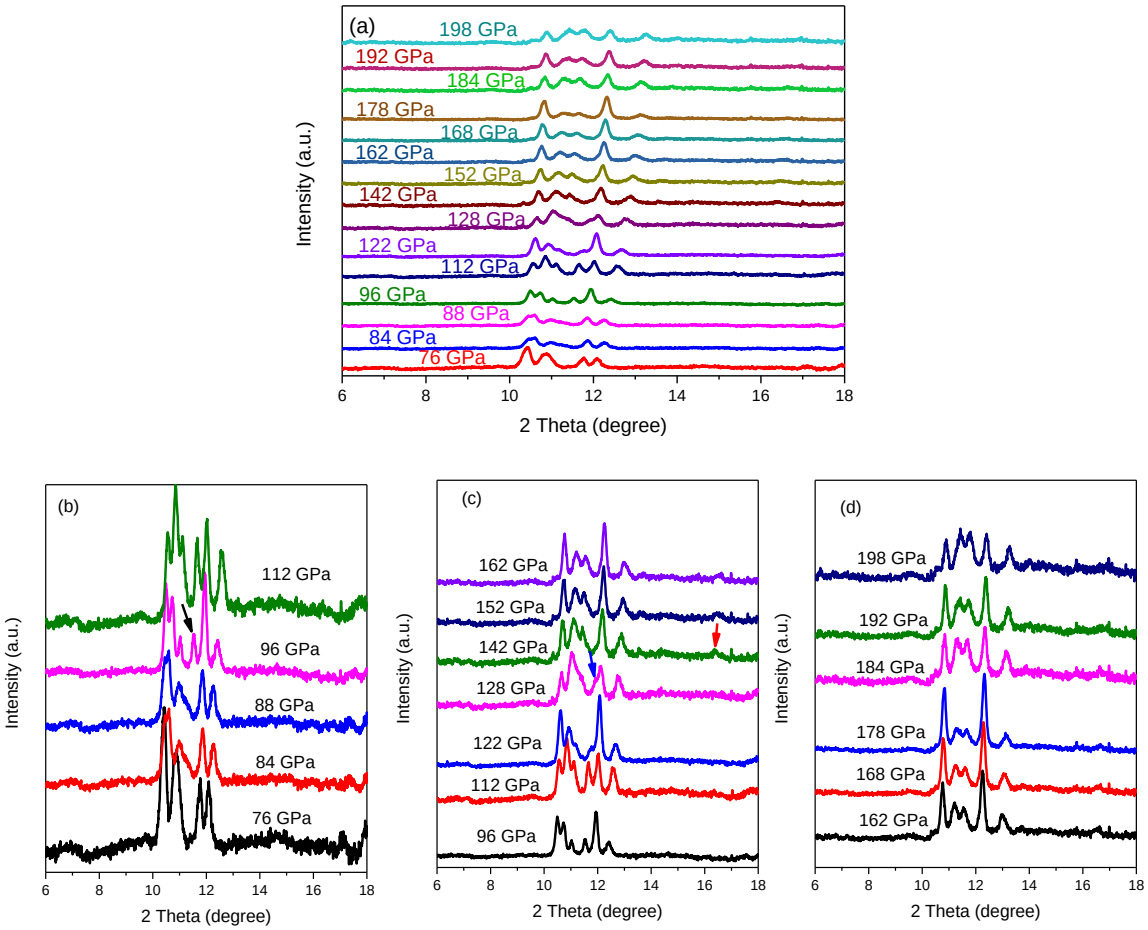

Fig. S2 (a~d) The *in-situ* high pressure synchrotron x-ray diffraction experiments were carried out at BL10XU, SPring-8, Japan, with the wavelength of 0.4126 Angstrom. As shown in Fig. S2(b), a new peak at around 2 Theta = 11.5 degree, marked by black arrow in the diffraction pattern collected at 96 GPa, suggests a phase transition from the Sc II to Sc III phase. Fig. S3(c) demonstrates a phase transition from Sc III to Sc IV occurs at about 142 GPa, which is suggested by the peak appearance at 2 Theta at about 16.4 degree and the peak disappearance at about 11.9 degree marked by red and blue arrows, respectively. In the pressure range from 142 to 198 GPa, the Sc IV phase is stable as seen in Fig. S2(d).

II. Theoretical calculations

The electronic structure, phonons and electron phonon coupling on Sc V phase at 240 GPa were calculated using the Quantum Espresso (QE) package [S1] with the Optimized Norm-Conserving Vanderbilt (ONCV) PBE [S2] pseudopotential for Sc obtained from the QE website. The energy cutoff is 80 Ryd and the density cutoff is 640 Ryd. The *k* point sets for SCF and charge density calculations were 12*12*6 and 24*24*12, respectively. Th *q*-point set for phonon calculations was 6×6×6. The computed band structure, phonon density of states (vDOS) and Eliashberg function ($\alpha^2F(\omega)$) are shown in Fig. S3. The results are in very good agreement with those reported in ref. 32. It is interesting to note that the profiles of the vDOS and $\alpha^2F(\omega)$ are very similar, as in the typical elemental superconductor Nb.

The valence orbital occupation of S V at 240 GPa were calculation with the ADF suite [S3] using the PBE functional on the optimized structure described above. A triple zeta augmented with polarization functions(TZ2P) basis set for Sc was used.

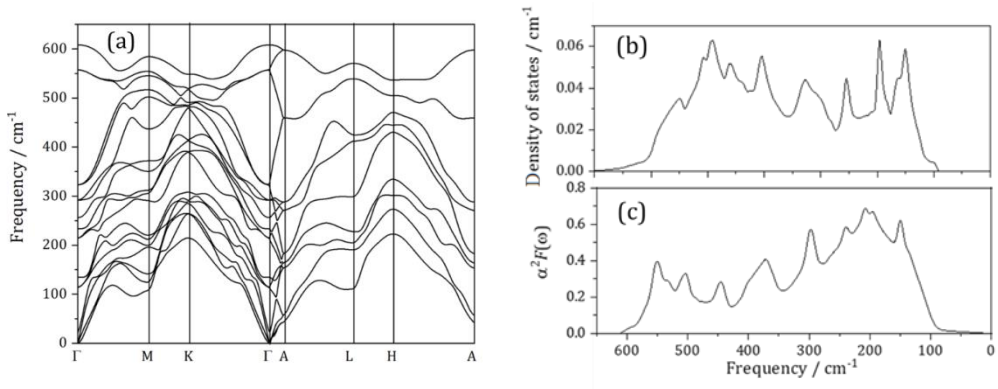

Fig. S3 (a-c) Calculated phonon structure, phonon vibrational density of states and Eliashberg function for ScV phase at 240 GPa.

References

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