Supplemental Material for

High-pressure synthesis and neutron scattering study of tantalum hydride $TaH_{1.23(5)}$, and a tantalum polymorph with A15-type structure

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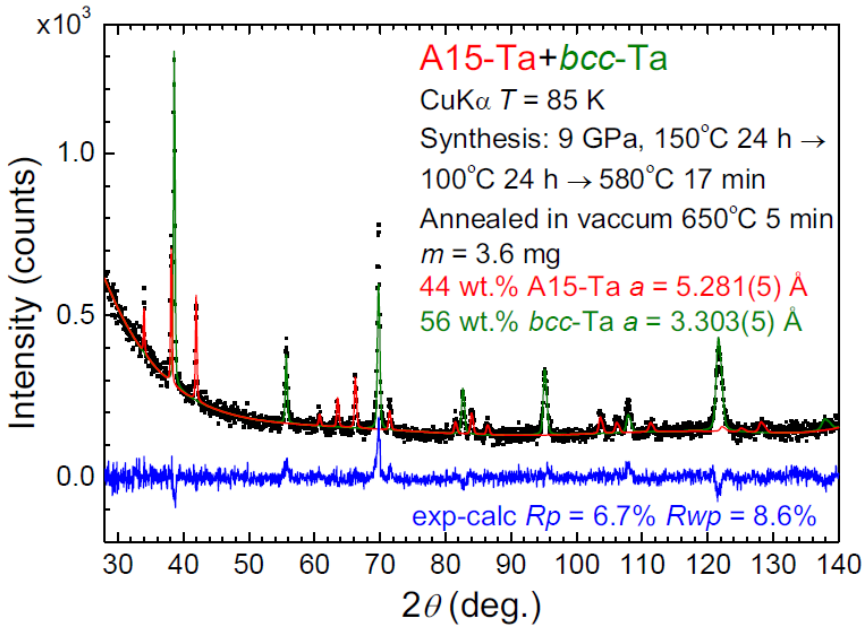

Fig. SM1. Powder X-Ray diffraction pattern of the A15-Ta + *bcc*-Ta sample produced after the removal of hydrogen from A15-TaH_x by annealing in vaccum at 650°C, and the results of the Rietveld fit. The contributions from A15-Ta and *bcc*-Ta are shown by the red and green curves, respectively, and the blue curve is the fit residual. Intensity variations from *bcc*-Ta mostly result from insufficient averaging over grain orientations due to small sample mass.

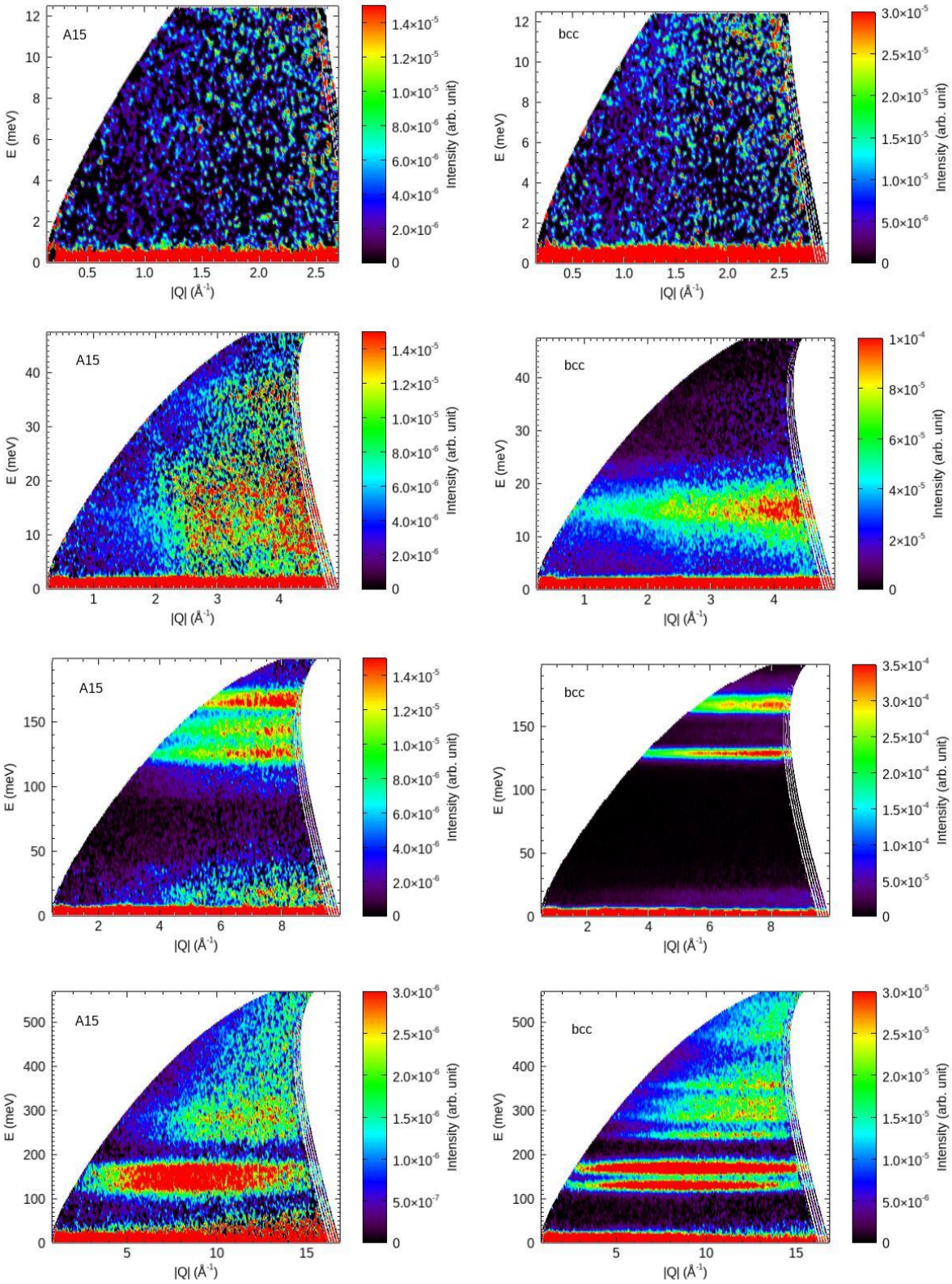

Fig. SM2. (Q,E) contour plots of $S(Q,E)$ spectra of 55 wt.% A15-$TaH_{0.95}$+45 wt.% bcc-$TaH_{0.76}$ (left) and *bcc*-$TaH_{0.85}$ (right) measured at T = 4 K using the SEQUOIA spectrometer with the incident neutron energies of E_i = 18, 50, 210 and 600 meV (top to bottom). The background from sample holder has been measured separately and subtracted from each dataset.

Table SM1. Lattice parameters of presently known tantalum polymorphs and hydrides. The lattice parameters of solid solutions of hydrogen in *bcc*-Ta are reviewed elsewhere [22, 48].

Material	Crystal structure	Temperature, K	Lattice parameters, Å	Reference
Ta	*bcc*	293 85	3.3029(2) 3.299(1)	[42]
β-Ta	β-U-type(*tP*30)	293	a = 10.194(3) c = 5.313(2)	[43]
$TaH_{0.89(3)}$	In-type(*tI*2) with long period ordering of H atoms in tetrasites	100	a = 3.405(1) c = 3.453(1)	[24]
hcp-$TaH_{2.2(1)}$	*hcp* with hydrogen in tetra- and octasites	85	a = 3.223(1) c = 5.143(2)	[21]
*cI*16-TaH_3	High pressure Li-type(*cI*16, distorted *bcc*), hydrogen in tetrasites	293	7.44(2)	[26]
A15-$TaH_{1.23(5)}$	A15, hydrogen in tetrasites	85	5.510(3)	present
A15-$TaH_{1.11(5)}$ annealed at –68°C	A15, hydrogen in tetrasites	85	5.480(3)	present
A15-$TaH_{1.03(5)}$ annealed at 50°C	A15	85	5.475(5)	present
A15-$TaH_{1.04(5)}$ annealed at 100°C	A15	85	5.477(5)	present
A15-$TaH_{0.94(5)}$ annealed at 200°C	A15	85	5.459(5)	present
A15-$TaH_{0.43(5)}$ annealed at 300°C	A15	85	5.328(5)	present
A15-Ta annealed at 400-600°C	A15	293 85	5.295(5) 5.281(5)	present