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High Pressure – High Temperature Polymorphism in Ta: Resolving an Ongoing Experimental Controversy

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Abstract

Phase diagrams of refractory metals remain essentially unknown. Moreover, there is an ongoing controversy over the high pressure (P) melting temperatures of these metals: results of diamond anvil cell (DAC) and shock wave experiments differ by at least a factor of two. From an extensive *ab initio* study on tantalum we discovered that the body-centered cubic phase, its physical phase at ambient conditions, transforms to another solid phase, possibly hexagonal omega phase, at high temperature (T). Hence the sample motion observed in DAC experiments is not due to melting but internal stresses accompanying a solid-solid transformation, as explained in more detail in our work. In view of our results on tantalum and previous work on molybdenum, as well as other published data, it is highly plausible that high- PT polymorphism is a general feature of Groups V and VI refractory metals.

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There is an ongoing controversy over the high-pressure melting of Groups V and VI refractory metals that began with the first diamond-anvil-cell (DAC) measurements of the melting temperatures of V, Ta, Cr, Mo, and W nearly a decade ago [1]. In the DAC experiments, melting at a given pressure, P , is assumed to coincide with the onset of sample surface motion as the temperature, T , is raised by laser heating of the sample. Melt temperatures, T_m , as determined by this technique, are consistently lower than those obtained from shock wave (SW) experiments, wherein T_m is determined from a calculated equation of state using the measured pressure and density at which the longitudinal sound speed in the equilibrium shock state (Hugoniot) suddenly drops with increasing pressure because of the loss of shear strength on melt. The discrepancy between the DAC and SW values of T_m at high P is at least a factor of two: for V at ~ 225 GPa, $T_m \sim 3000$ K from the extrapolated DAC melt curve [1], as compared with a SW value of $T_m \sim 7800$ K [2]; for Ta at ~ 300 GPa, an extrapolated DAC [1, 3] $T_m \sim 4000$ K versus a SW [4] $T_m \sim 10000$ K; and for Mo at $P \sim 400$ GPa, an extrapolated DAC [1, 5] $T_m \sim 4000$ K versus a SW [6] $T_m \sim 10000$ K.

The refractory metals have a characteristic body-centered cubic (*bcc*) structure under ambient conditions, and consequently, all but one of the theoretical efforts to resolve this DAC/SW melting controversy have been based on comparisons of *bcc* melt curves [7]. The exception is our previous work on Mo [7, 8], where we considered other solid phases. Using *ab initio* density functional theory (DFT) methods, we found that the face-centered cubic (*fcc*) structure melts at a higher temperature and is hence more stable than *bcc* at pressures exceeding roughly 150 GPa. This does not prove that the *fcc* structure is the most stable phase there, only that it is more stable than *bcc*; indeed, there is evidence [8] that other crystal structures may be more stable than *fcc* at high P - T , and therefore may melt at even higher temperatures than *fcc*. In any case, our calculated *fcc* melt curve is consistent with the high observed SW T_m of Mo, and moreover, our estimated *bcc*-*fcc* phase boundary at low pressure is consistent with the DAC melt curve, as well as with the observed break in the Hugoniot sound-speed curve at ~ 200 GPa prior to shock melt [6]. On that basis, we proposed [7] that the build-up of internal non-hydrostatic stresses accompanying a solid-solid phase transformation is responsible for the observed material flow of Mo at high P - T in the DAC experiments. Such an explanation could also apply to the other refractory metals.

In addition to sample surface flow, the disappearance of some *bcc* X-ray diffraction lines at the DAC melt temperatures in subsequent experiments on Ta [3] and Mo [5] contributed to

the conclusion that melting had occurred. However, the inverse problem of deducing structure from diffraction patterns is non-trivial, and can easily lead to erroneous conclusions. Indeed, the claimed discovery of a new phase of Zr, namely, Zr glass [9], in the vicinity of the *bcc* to hexagonal omega (hex- ω) phase transition boundary was later retracted [10]. The initial conclusion was based on the disappearance of some solid-like X-ray diffraction lines, but a subsequent more careful analysis revealed that the disappearance of the lines occurred because of rapid crystal growth at temperatures above the phase transformation. Similarly, rapid recrystallization, or the growth of a new crystal phase, can occur in DAC melting experiments under the *P-T* conditions close to those of a solid-solid transition. In particular, in their analysis of the DAC experiments on Mo [11], Ross *et al.* observed permanent rapid recrystallization of the sample “with a dramatic change of the Bragg peak intensity, from one solid-like diffraction pattern to the next, probably due to locally preferred orientation nucleation during recrystallization;” here “the next” solid-like pattern must be that of an ingrowing phase more stable than *bcc*.

A recent study by Wu *et al.* [12], motivated in part by the possibility that shear stresses play a key role in the structural transformations occurring in the DAC, performed molecular dynamics (MD) simulations of Ta with a quantum-based, multi-ion MGPT (model generalized pseudopotential theory) interatomic potential [13]. They found a shear-induced transformation from *bcc* to a partially disordered, partially crystalline structure, and the *P-T* dependence of the transformation coincides closely with the DAC melt curve. They interpreted this transformation as a Bingham-like plastic flow, where the shear-dependent flow character is linked to a flat energy landscape associated with the geometric distortion of {110} planes, and as such, it is likely tied to high *P-T* polymorphism. In this regard, previous MGPT studies at high *P-T* conditions in Ta have shown both a substantial elastic softening of the *bcc* structure [14], which is presumably a precursor to any phase transition in the solid, and the appearance of a mechanically stable and energetically competitive cubic *A15* phase [15]. Moreover, as discussed below, we have carried out both *ab initio* and MGPT MD simulations of high-pressure Ta melting from different phases, and each predicts the existence of a solid phase more stable than *bcc* at high *P-T*.

We now turn to our present *ab initio* study of Ta, which conclusively demonstrates that Ta is polymorphic at high *P-T*. Crystal structures typical of the transition-metal series, namely, *bcc*, *fcc*, hexagonal close packed (*hcp*), and double-*hcp* (*dhcp*) were considered, as

were several structural arrangements related to *bcc*, specifically, the hex- ω and cubic *A15* phases, and also the α -U lattice, which is related to the close-packed structures. Our DFT calculations of the electron and phonon spectra, as well as our *ab-initio* MD simulations of Ta, were performed in the framework of the frozen-core all-electron projector augmented wave method [16], as implemented in the program VASP [17]. The phonon calculations were carried out in the framework of the supercell approach (see ref. [18] for details). To maintain high accuracy we used $3\times 3\times 3$ supercells. The energy cut-off was set to 400 eV. Exchange and correlation effects were treated within the generalized gradient approximation [19]. The semi-core $4p$ states of Ta were treated as valence. The integration over the Brillouin zone was based on the Monkhorst-Pack scheme [20]. Relaxation of the structural parameters and force calculations were carried out according to the Methfessel-Paxton scheme [21], while total-energy calculations were performed using the tetrahedron method with Blöchl corrections [22].

The calculations at zero temperature (Fig. 1) show that *bcc* is the lowest-energy solid structure over the entire pressure range considered, 0 – 1 TPa. At zero pressure the hex- ω and *A15* phases have excess energies of about 240 meV/atom and 70 meV/atom, respectively, which increase steadily with compression, reaching 850-890 meV/atom at 1 TPa. The behaviors of the *fcc*, *hcp*, and *dhcp* structures are different. Their excess energies at zero P are tightly clustered around 300 meV/atom. Under compression they increase and reach maxima of 740-795 meV/atom at 500-600 GPa, and then decrease with further compression to 640-700 meV/atom at 1 TPa. The α -U structure coincides with *bcc* upon relaxation. Interestingly, the *bcc* phase is the only mechanically stable phase among all those considered up to 1 TPa. The zero- T phonon spectra of the other phases contain imaginary frequencies at all pressures considered, which implies their mechanical instability. Besides, by displacive deformation of the internal and/or external structural parameters, each of them can be transformed into *bcc*. With increasing pressure, the mechanical instability of each of these phases is enhanced, which is in accord with the overall increase in the total energy differences with pressure, but at sufficiently high temperature, these phases become mechanically stable, due to a combination of ion-thermal and electron-thermal effects, and hence thermodynamically they are either stable or metastable.

We next performed a suite of finite temperature *ab initio* MD simulations of melting from the *bcc*, *fcc*, *hcp*, *dhcp*, *A15*, and hex- ω phases of Ta using the so-called Z method [23]. The

system sizes, simulation times, etc. were the same as those used in our previous simulations of Mo melt [7]. We find that all of the solid phases considered in Ta become mechanically stable at high T . They all have normal melt curves (solid-liquid coexistence lines), three of which are shown in Fig. 2, along with the experimental DAC data [3], and our estimated shock Hugoniot. Not shown are the $A15$, fcc , and $dhcp$ melt curves: $A15$ is indistinguishable from bcc within the error bars; fcc is close to hcp ; and $dhcp$ is the lowest curve of all. For the sake of clarity, the Z -isochores from which the melt curves are determined are not shown in Fig. 2, although they are typical and similar to those seen in Fig. 3. Our bcc melt curve is close to the previous *ab initio* result of Taioli *et al.* [24] and about 20% lower at 500 GPa than the result of the MGPT MD simulations presented below.

In Fig. 2, only the hex- ω melt curve crosses the bcc melt curve – the intersection point is at about 70 GPa and 5650 K; hence, the hex- ω phase of Ta is more stable than bcc at higher pressures. The hex- ω and bcc structures are closely related: in the hexagonal representation of the unit cell, both have three atoms per cell, and the hex- ω phase results when the two atomic planes of the bcc phase collapse into a common plane. The c/a ratio of the hex- ω phase of Ta as a function of pressure is shown in the inset of Fig. 1. It is seen that, with increasing P , it tends to the “ideal” bcc value of $\sqrt{3/8} \approx 0.6124$.

With regards to the bcc -hex- ω phase boundary in Ta, we have used the Clausius-Clapeyron formula to estimate its slope near the bcc -hex- ω -liquid triple point: $-(100-120)$ K/GPa. If approximated by a straight line, this phase boundary would cross the Hugoniot at ~ 100 GPa and 2400-2500 K (see Fig. 2); below we compare this prediction with Hugoniot sound speed data. The shock melting point, that is, the intersection of the Hugoniot and the hex- ω melt curve, is at $(P, T) \sim (300 \text{ GPa}, 11500 \text{ K})$. Our calculated T_m is thus about 15% higher than the original SW estimate of 10000 K [4].

In addition to our *ab initio* simulations of the high P - T solid phases of Ta, we also carried out a series of MGPT MD simulations of the bcc , fcc , and $A15$ phases of Ta using the Z method. The calculations were carried out at a number of volumes from $23 \text{ \AA}^3/\text{atom}$ ($P \sim -30 \text{ GPa}$ at $T = 0$) down to $10 \text{ \AA}^3/\text{atom}$ ($P \sim 350 \text{ GPa}$ at $T = 0$). We used a 250-atom bcc supercell obtained by $5 \times 5 \times 5$ multiplication of a 2-atom unit cell, a 256-atom fcc supercell ($4 \times 4 \times 4$, 4-atom unit cell), and a 216-atom $A15$ supercell ($3 \times 3 \times 3$, 8-atom unit cell). The time step was 1 fs to minimize numerical errors. The system was equilibrated for 8000 timesteps, after which the averages were accumulated. All MGPT results for Ta, either

presented or cited, were calculated with version 4.0 of the MGPT potential (also known as Ta4 or Ta-IV), also used by Wu *et al.* [12]. In Fig. 3, we show three pairs of *bcc-fcc* *Z*-isochores (16, 12, and 10 Å³/atom) and one *A15* *Z*-isochore (10 Å³/atom). To within the statistical errors, the high pressure *A15* and *bcc* *Z*-isochors are indistinguishable, as is the case for their *ab initio* counterparts. The fact that the *A15* and *bcc* melt curves are very close, which implies nearly equal free energies at high *T*, is consistent with the appearance of *A15* during the intermediate stages of previous MGPT MD simulations of the solidification of Ta [15]. The present calculation shows unambiguously that the *fcc* melting curve lies above that of *bcc* at the highest melting pressure considered, i.e., 470 GPa: the difference of about 1000 K in the melting temperatures lies outside any statistical error. Based on accurate fits to the MD data using the Simon functional form, the *bcc-fcc* intersection occurs at about 15 GPa (and 4300 K). The *fcc* phase is unquestionably more stable than *bcc* at high *P-T*. As regards the *bcc-fcc* phase boundary in these MGPT calculations, it is certainly above 5000 K at 150-170 GPa, which were the *P-T* conditions in the MGPT Ta solidification simulations [15]. In those simulations, the *fcc* phase never appeared, only *bcc* and *A15*, and because of the large system size, approximately 10 million atoms, the *fcc* phase should have been present if it were mechanically stable.

We now show that our linearly extrapolated *ab initio* *bcc-hex- ω* phase boundary is in excellent agreement with Hugoniot sound speed data on Ta. The earliest data set consisted of twelve points, eleven of which were published [4]; these are shown in Fig. 4 as blue circles. The twelfth unpublished datapoint (magenta star) was recently provided to us [25]. With the addition of the datapoint from [26] (red box), and the three most recent datapoints from [27] (green diamonds), Fig. 4 displays all available Ta Hugoniot sound speed data (ambient sound speeds are also shown as brown triangles). The discontinuity in the longitudinal sound velocity at ~ 100 GPa is very possibly the signature of a solid-solid phase transformation. Remarkably, the intersection of our extrapolated *bcc-hex- ω* phase boundary and the estimated Hugoniot in Fig. 2 is also located at about 100 GPa. In order to bring our *ab initio* MD results into full correspondence with the sound speed data, calculations of the high *P-T* elastic moduli of the solid phases of Ta, *hex- ω* in particular, need to be carried out. Previous MGPT calculations of high *P-T* elastic moduli and longitudinal sound speeds in *bcc* Ta [14] are in good accord with the experimental data shown in Fig. 4 below 100 GPa and also above 150 GPa.

The present investigation confirms that the *bcc* structure of tantalum is supplanted by another solid phase at high pressures and temperatures. Although our calculations on Ta do not rule out the possible existence of additional high-pressure phases more stable than any considered in this study, the hexagonal omega phase of Ta predicted by our *ab initio* approach is a very likely candidate for the high *P-T* structure of Ta above ~ 70 GPa. We note that this phase was observed in a shock-recovered sample of Ta by Hsiung and Lassila [28], although the material was shocked to only 45 GPa and ~ 550 K, where, according to Figs. 1 and 2, *bcc* is the stable phase. Also, the three Group IV metals, Ti, Zr, and Hf, the neighbors of V, Nb, and Ta in the periodic table, transform into the hex- ω phase at high pressure and may melt from this phase. In any case, the discovered polymorphism in Ta makes a solid-solid transformation from *bcc* to a higher-*T* phase, possibly the hex- ω phase, a viable mechanism for the observed material flow in the DAC experiments. The flow occurs because of the rising internal stresses accompanying the solid-solid transformation and the thermal stresses associated with laser heating. We also point out that the hex- ω phase was previously found by us to be more stable than *bcc* at high *P-T* for Mo [8], and that it was shown in refs. [29] that W can exist in the hex- ω structure. Hence, this phase may also be present in Group VI metals. As another example of Group VI high *P-T* polymorphism, Hugoniot sound speed measurements on tungsten [30] indicate a possible solid-solid phase transformation on the Hugoniot at a pressure of ~ 200 GPa, well below shock melting at ~ 400 GPa. Thus, it is highly plausible that high *P-T* polymorphism is a general feature of the Groups V and VI refractory metals, and transformations from *bcc* to the higher *T* structure are responsible for the low temperature flows observed in DAC experiments on refractory metals.

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Figure captions

Figure 1. Pressure dependence of the $T = 0$ enthalpies of the *fcc*, *hcp*, *dhcp*, *A15*, and *hex- ω* structures of Ta relative to the $T = 0$ enthalpy of the *bcc* phase; pressure dependence of the c/a -ratio of the *hex- ω* at $T = 0$ K (inset).

Figure 2. *Ab initio* melt curves of the *bcc* (blue), *hex- ω* (green), and *hcp* (brown) phases of Ta, along with the experimental data of ref. [3], our estimated shock Hugoniot (long dashed line), and our approximate *bcc-hex- ω* phase line (short dashed line).

Figure 3. Z-isochores for *bcc*, *fcc*, and *A15* Ta at volumes of 16, 12, and 10 Å³/atom obtained by MGPT MD. The intermediate descending part of the Z-isochore corresponds to the melting process, its lowest point being the true melt point [23]. Dashed lines are our best fits to the *bcc* (blue) and *fcc* (green) results.

Figure 4. Hugoniot sound speed data on Ta. See the text for references. Dashed lines are a guide to the eye only. However, the low- P upper segment and the whole lower line closely follow, respectively, $c_L \equiv \sqrt{(B + \frac{4}{3}G)/\rho}$ and $c_B \equiv \sqrt{B/\rho}$ for *bcc*-Ta.

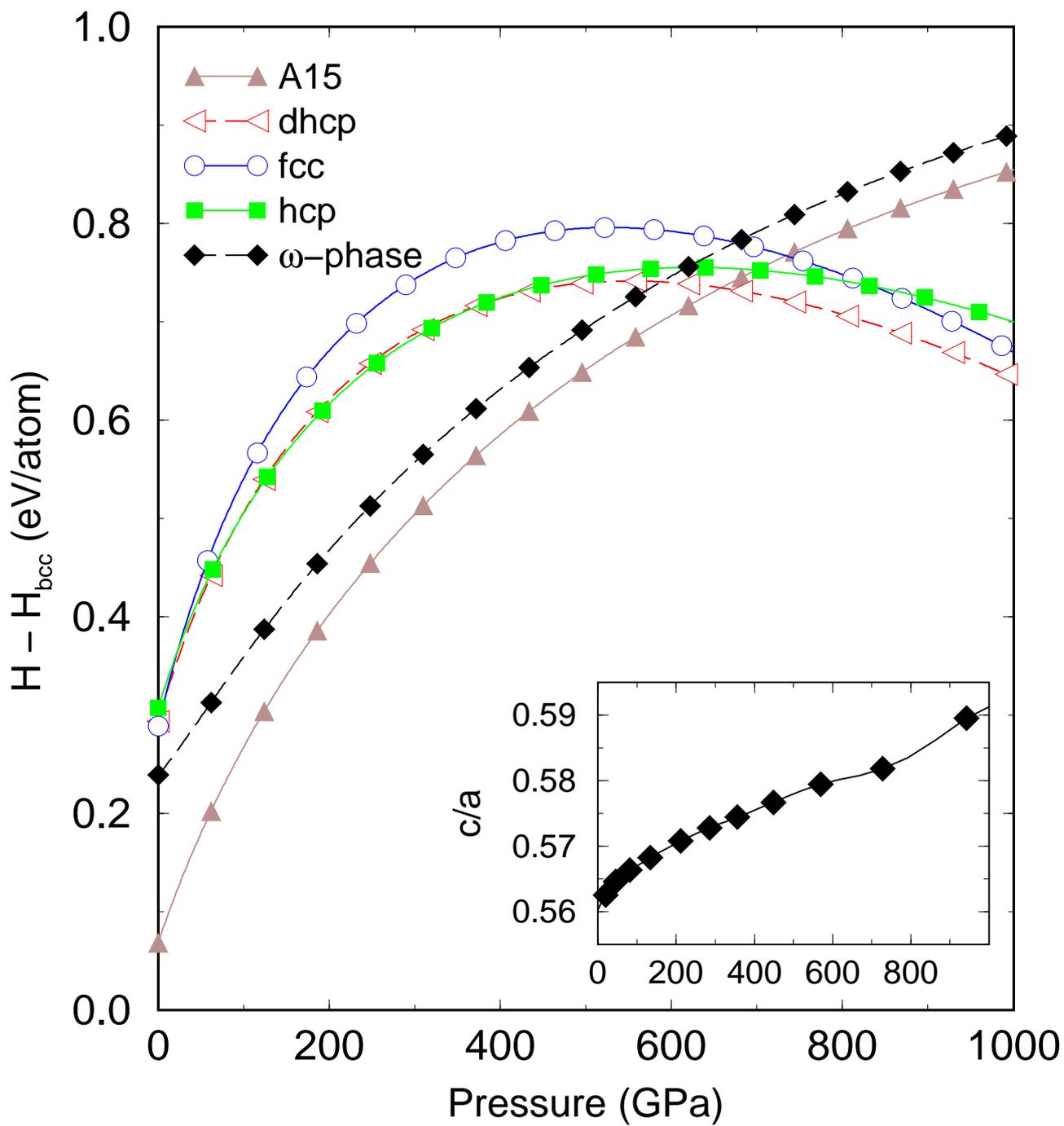


Fig. 1

Melting curves: omega (green), bcc (blue), hcp (brown)

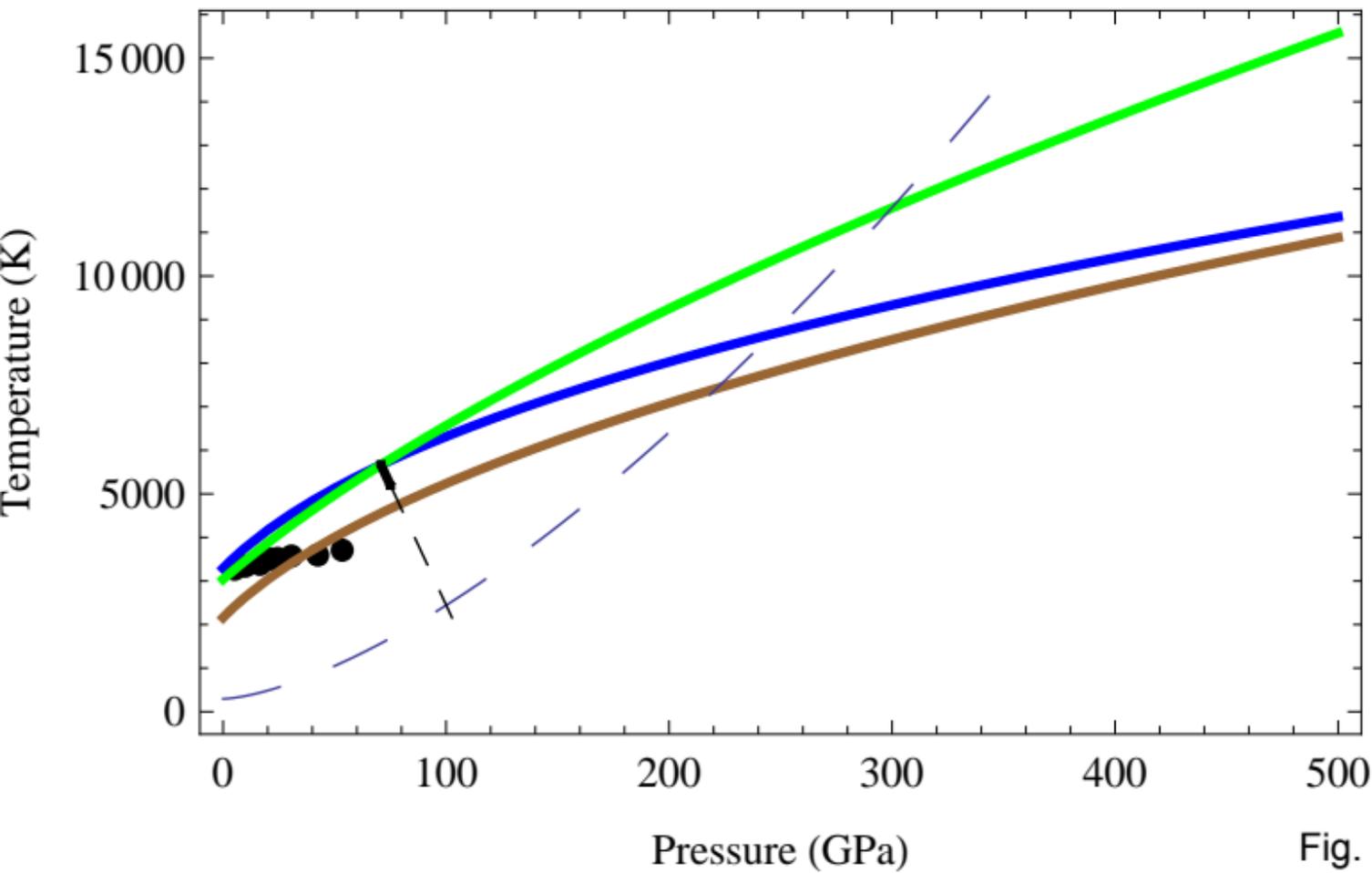


Fig. 2

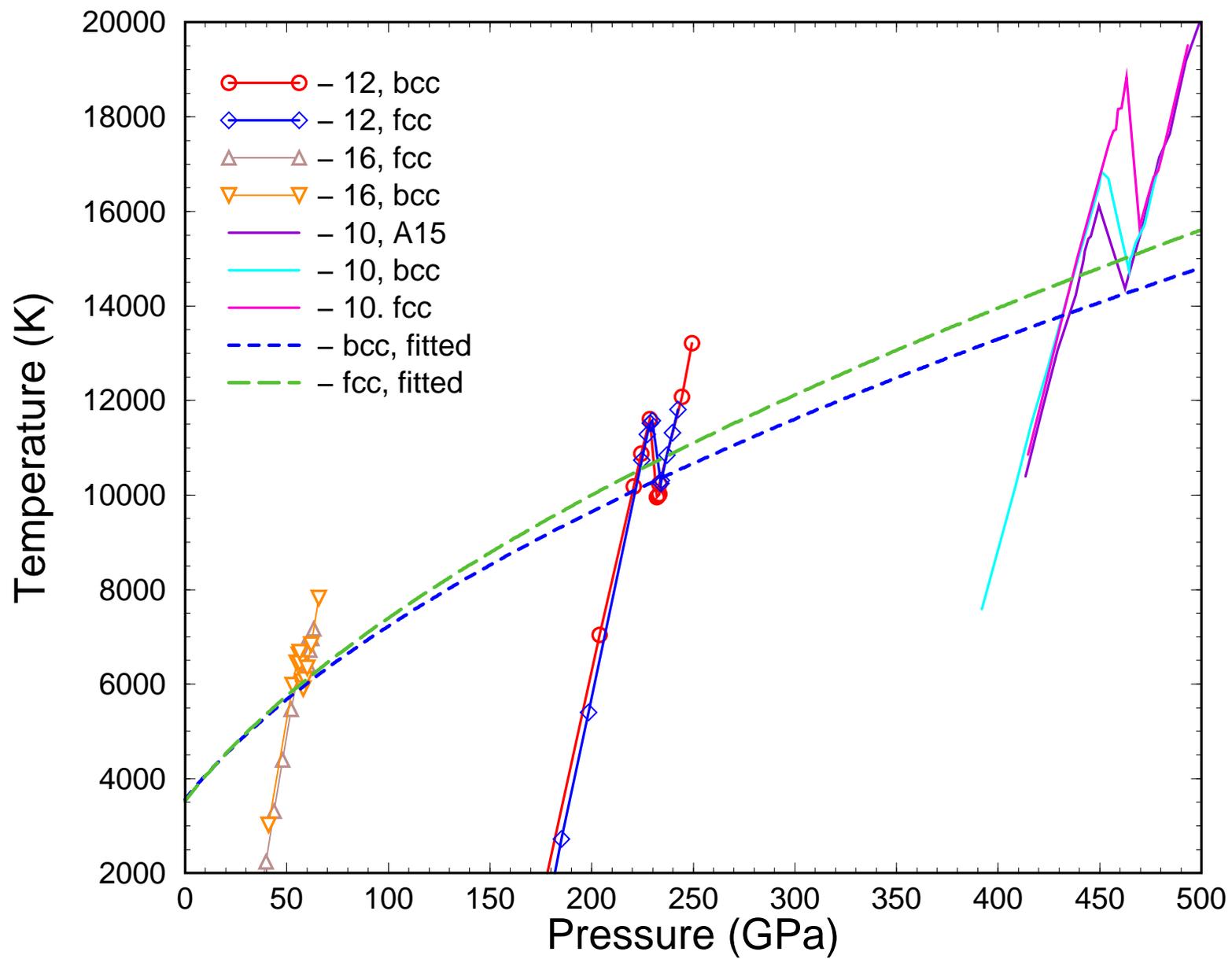


Fig. 3

Tantalum

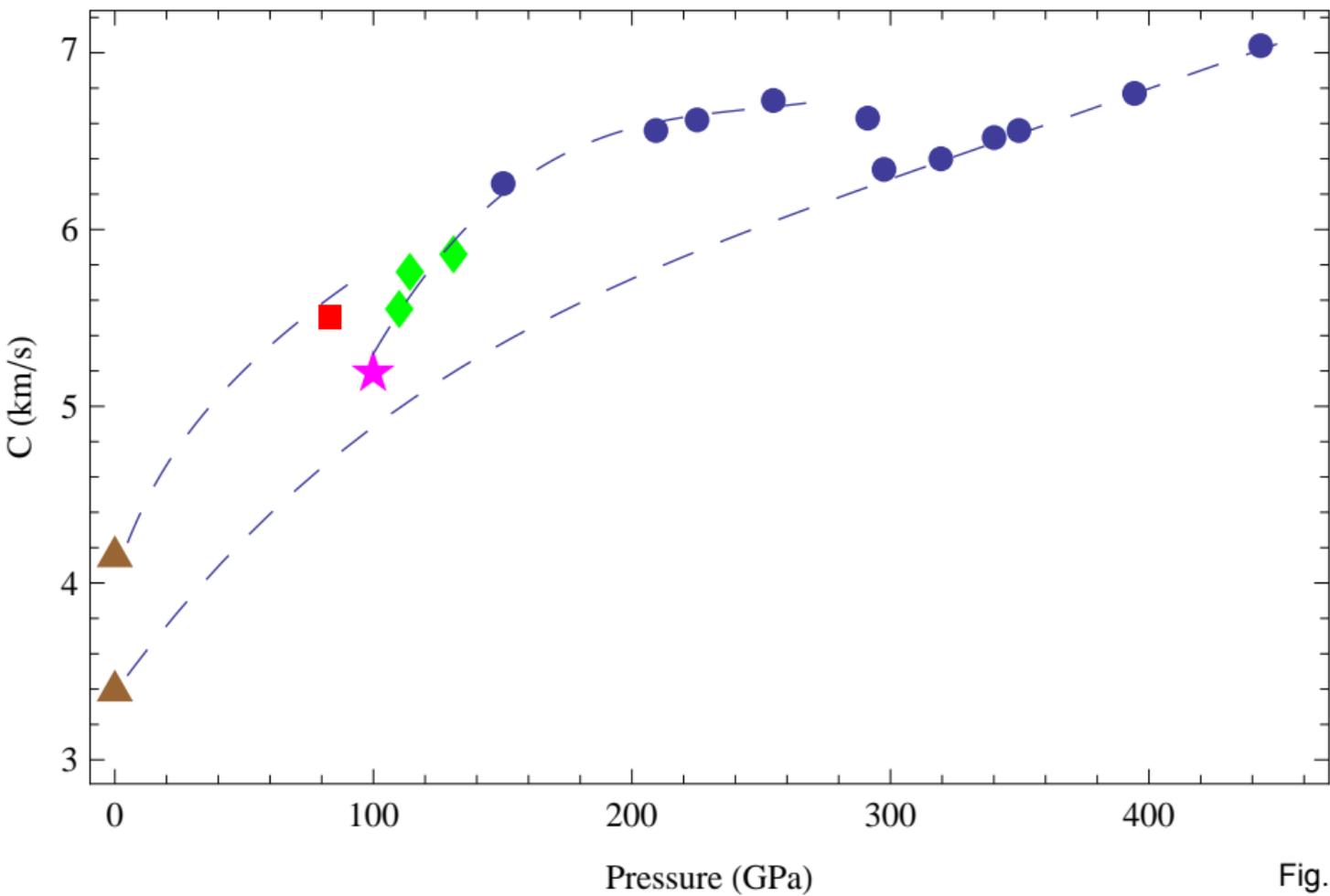


Fig. 4