Recent *Ab Initio* Studies of Phase Diagrams: Al, Tl, Mo, and W

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We present the results of our recent studies of the phase diagrams of aluminum, thallium, molybdenum and tungsten. These studies are based on *ab initio* quantum molecular dynamics simulations using complete Z methodology [1] (the combination of direct and inverse Z methods the brief overview of which will be given) as implemented with VASP (Vienna *Ab initio* Simulation Package).

It is firmly established experimentally that both Al and Tl are polymorphic (multi-phase) substances. However, the melting properties of their high-pressure phases, body-centered cubic (bcc) for Al and face-centered cubic (fcc) for Tl, have never been studied, either experimentally or theoretically. Likewise, the theory suggests that both Mo and W are polymorphic, although their polymorphism has not been detected in experiments yet.

In the course of our theoretical study we have caluclated the melting curves of the low- and high-pressure phases of the four materials using the direct Z method. The intersection of the low-*P* and high-*P* melting curves gives the corresponding triple point. The solid-solid phase transition boundaries were determined based on the available experimental data and the VASP simulations of the solidification of liquid into different final solid states on both sides of the phase boundary using the inverse Z method. The phase diagram of Tl is shown in *Figure 1* as an example of our findings. The corresponding experimental data points come from [2]. The bcc-fcc-liquid triple point is found to be at (*P*, *T*) = (10 GPa, 1015 K).

As for the remaining three phase diagrams that will be presented during the talk, the fcc-bcc-liquid triple point in Al is predicted to occur at around 200 GPa. The phase diagrams of Mo and W are topologically equivalent, each having two stable solid phases over the corresponding *P*-*T* regions, specifically, bcc and double hexagonal close-packed (dhcp). The bcc-dhcp solid-solid phase transition boundaries extend from $T = 0$ and $P \sim 650$ GPa for Mo, and from $T = 0$ and $P \sim 1050$ GPa for W, to the corresponding bcc-dhcp-liquid triple points at higher *P*.

Our *ab initio* studies that we will present during this talk fill out the gaps in the knowledge of the four phase diagrams. Our theoretical techniques can be applied to the study of other phase diagrams that are currently unknown or known poorly.

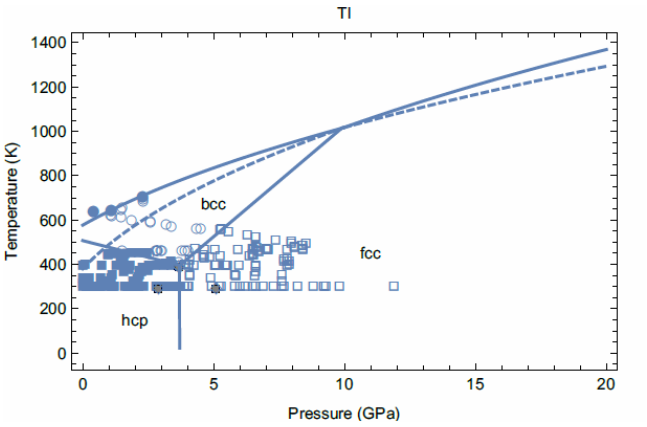

Figure 1. The phase diagram of thallium that combines experimental data points and *ab initio* phase boundaries

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References

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