

Abstract Submitted  
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**Z methodology for phase diagram studies: tantalum and platinum as examples** LEONID BURAKOVSKY, DEAN PRESTON, SHAO PING CHEN, DANIEL SHEPPARD, Los Alamos National Laboratory, Z- TEAM — Z methodology is a novel technique for phase diagram studies. It combines direct Z method for the calculation of melting curves, and inverse Z method for the calculation of solid-solid phase boundaries. Relative solid phase stability is studied by comparing melting curves of different solid phases to determine which one is the highest, and thus which of the corresponding solid phases is the most stable. is accomplished using direct Z method. Subsequently, solid-solid phase boundaries can be determined by freezing liquid into the most stable solid phases on both sides of the phase boundary. Inverse Z method represents the implementation of this approach in terms of ab initio molecular dynamics using VASP package. We will discuss the application of Z methodology to the study of the phase diagrams of tantalum and platinum, and compare our results to the most recent experimental data.

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