Ab Initio Study of Random Hexagonal Close-Packed Phase in Platinum

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Random hexagonal close-packed (rhcp) phase is a solid structure that has recently been widely discussed in the literature. It is realized when structures with different stacking sequences (AB . . . for hcp, ABC . . . for fcc, ABAC . . . for dhcp, ABCACB . . . for thcp, ABCBCACAB . . . for 9R, etc.) generally called hexagonal polytypes are energetically very close. Hence, the energy cost of forming a stacking fault between two such structures is virtually zero. Consequently, the actual layer stacking could be non-periodic and, in principle, random, thus forming rhcp. Rhcp was first introduced for hard-sphere colloids [1], and later on has been proposed for several elemental solids, e.g., Fe, Ir, Pt, Ag, and Au. For Pt, rhcp was first proposed in our previous Z-methodology-based theoretical study [2]. Here we use the technique of three-phase *ab initio* quantum molecular dynamics simulations to demonstrate the appearance of rhcp for Pt, and to determine the phase boundary that separates rhcp from the ambient face-centered cubic (fcc) phase of Pt on its phase diagram. These simulations consist in evolving a system containing layers of two different hexagonal polytypes separated by liquid regions until the system reaches its final equilibrium state. The example of such a three-phase simulation is shown in Figure 1: an initial system containing layers of fcc and 9R evolves towards the final rhcp state. It then appears that the results of the most recent experimental study on the melting curve of Pt [3] map out the melting curve that virtually coincides with the fcc-rhcp phase boundary that we present here, see Figure 2. The reasons for misinterpreting the fcc-rhcp solid-solid transition as melting will be briefly discussed.

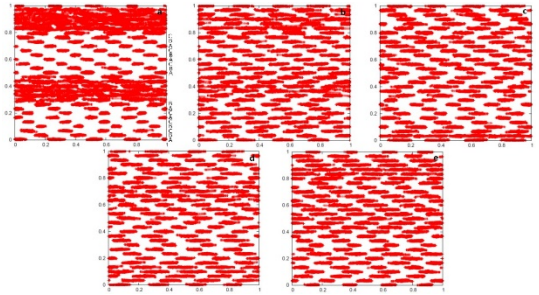

Figure 1: Example of a three-phase *ab initio* quantum molecular dynamics simulation.

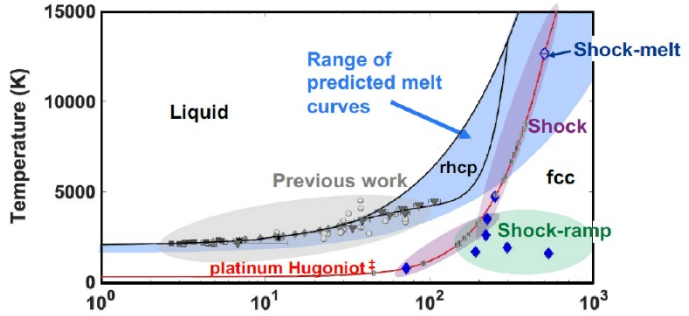

Figure 2: The phase diagram of Pt according to [4].

References

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