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Melting curve of Ta from the modified Z method in molecular dynamics simulation¹ WANG SHUAICHUANG, LIU HAIFENG, ZHANG GONGMU, SONG HAIFENG, TANG LI, IAPCM (Institute of Applied Physics and Computational Mathematics), IAPCM TEAM — Our recently proposed modified Z method to calculate the melting curve of metals has an obvious feature that a system can run naturally into its steady solid-liquid coexistence state from a perfect solid configuration in one running process. The method has been proved to be successful for face-centered cubic metals. Now we examine its validity for the melting curve of body-centered cubic metals, Ta as an example. A steady solid-liquid coexistence state can still be achieved for a system with only about 1000 atoms. The melting temperature and pressure results of Ta, extracted from the coexistence state, are in good agreement with those of the two-phase method in the literature.

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