Melting curves of Zr and Hf: estimates from *ab initio* calculations and pulse-heating experiment

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In this work we present the melting curves of hafnium and zirconium obtained using quantum molecular dynamics calculations. The mean-square displacements computed during ab initio simulations of a crystal phase are used to reconstruct the melting curve according to the Lindemann criterion. The resulting Zr melting curve shows a steeper slope in the low-pressure region compared to some recent diamond-anvil cell experiments but agrees with our previous estimate via the Clausius-Clapeyron relation. The slope for higher pressures is consistent with the experimental one.
Meanwhile, the change in melting temperature with increasing pressure found in pulse-heating experiments conducted by our experimental group also confirms the steep slope of the Zr melting curve at low pressures.
As for Zr, the Hf melting curve also has a similar steep initial slope being in agreement with our estimate from the Clausius-Clapeyron relation. Currently there are no data on the melting of Hf above atmospheric pressure, so we demonstrate the first ab initio estimate of the melting curve of Hf up to 225 GPa.
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