Initial Slope of a Melting Curve from Quantum Molecular Dynamics Simulations

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We present a technique for the calculation of the initial slope of a melting curve. The technique is based on *ab initio* quantum molecular dynamics (QMD) simulations. It consists in the determination of both the latent heat of fusion and volume change at melt, directly from QMD, and the use of the Clausius-Clapeyron relation to calculate the slope. The new technique will help in reconciliation of the thermophysical data on refractory metals, including thermal expansion, solid and liquid densities and enthalpies, and volume change at melt, which in many cases remain highly controversial. Two such cases, rhenium and osmium, are analyzed in detail. Both initial melting curve slopes obtained using the new technique are compared to those from direct QMD simulations of the corresponding melting curves, and to the available thermophysical data.